

CRYSTAL STRUCTURE OF THE LIGAND BINDING DOMAIN OF THE RETINOIC ACID-RELATED ORPHAN RECEPTOR ALPHA (ROR-ALPHA)

**FIELD OF THE INVENTION**

The present invention relates ROR $\alpha$  in crystallized form and methods for the preparation thereof. The invention further provides a three-dimensional model of ROR $\alpha$  and means for the design of ROR $\alpha$  modulators.

**BACKGROUND OF THE INVENTION**

The retinoic acid-related orphan receptor  $\alpha$  (ROR $\alpha$ ) is an orphan member of nuclear receptor protein family to which belong receptors such as retinoic acid receptor (RAR), peroxisome proliferator-activated receptor (PPAR), estrogen receptor (ER), vitamin D receptor (VDR) and thyroid receptor (TR). Like other members of the nuclear receptor family, ROR $\alpha$  exhibits a modular structure composed of several domains, among them a DNA-binding domain (DBD) and a ligand-binding domain (LBD). The latter displays low degree of homology with the LBD of T3R $\beta$  (25%), VDR (24%), RAR $\alpha$  (24%), PPAR $\alpha$  (24%) and RXR $\alpha$  (20%) from which X-ray structures have been solved. However, attempts to crystallize the LBD of ROR $\alpha$  have failed so far and no X-ray structure of ROR $\alpha$  was available. In addition, to this point, no ligand has been identified until now. Our understanding of the physiological role of the receptor would be greatly enhanced by the discovery of a natural ligand. Further, provision of the spatial organization would assist in the designing of agonists and antagonists of ROR $\alpha$ .

**SUMMARY OF THE INVENTION**

In one aspect, the present invention provides crystalline LBD of ROR $\alpha$ . In a related aspect the invention provides crystalline LBD of ROR $\alpha$  associated with a ligand.

In another aspect, the invention provides a set of co-ordinates representing the spatial organization of the LBD of ROR $\alpha$ . In a related aspect the invention provides a model of the LBD of ROR $\alpha$  comprising a set of co-ordinates embodying the structure of the LBD of ROR $\alpha$ . In another related aspect, this invention provides for a set of co-ordinates useful in drug design. In yet another related aspect, the invention provides for a method for identifying a substance binding to the LBD of ROR $\alpha$ , comprising providing a model embodying the structure of the LBD of ROR $\alpha$ , assessing the interaction of a candidate substance with said model, and selecting a substance which is predicted to interact with the LBD of ROR $\alpha$ . Substances identified by this method are also provided.

In a further aspect, the invention provides for a method for identifying a compound acting as agonist or antagonist of ROR $\alpha$  that binds to the LBD of ROR $\alpha$  comprising selecting a potential compound by performing rational drug design with one or more sets of atomic coordinates embodying the structure of the LBD of ROR $\alpha$ , contacting the potential compound with a LBD of ROR $\alpha$  and measuring the binding of the compound to the LBD of ROR $\alpha$ . Agonists and antagonists identified by this method are also provided.

In another aspect, the present invention provides for a method of screening for compounds interacting with ROR $\alpha$  comprising contacting ROR $\alpha$  with a candidate compound, measuring interactions between the candidate compound and ROR $\alpha$  in the absence of sterols, and selecting said compound if it interacts with ROR $\alpha$  in the absence of sterols. Preferred sterols are cholesterol or cholesterol derivatives. Compounds identified by this method are also provided.

In another aspect of the present invention, the use of ROR $\alpha$  for the screening of cholesterol related diseases is provided.

In yet another aspect the present invention provides a composition comprising LBD of ROR $\alpha$  and a sterol, preferably cholesterol or a cholesterol derivative. In a preferred embodiment, said composition is crystallizable.

#### **BRIEF DESCRIPTION OF THE TABLES AND FIGURES**

Table 1: Native crystal data and X-ray data statistics of LBD of ROR $\alpha$  in complex with cholesterol.

Table 2: Hg-derivative crystal data, X-ray data and heavy atom refinement statistics (for complex with cholesterol).

Table 3: Refinement statistics (for complex with cholesterol).

Table 4: shows effects of mutations preventing binding of cholesterol to ROR $\alpha$ .

Table 5: shows effects of fluvastatin on ROR $\alpha$  transcriptional activity.

Table 6: Effect of cholesterol and cholesterol derivative on ROR alpha transcriptional activity.

Table 7: Native crystal data and refinement statistics of LBD of ROR $\alpha$  in complex with cholesterol sulfate.

Table 8: Atomic structure coordinates for a representative structure of the LBD of ROR $\alpha$  in complex with cholesterol (numbering according to Swissprot P35398-1).

Table 9: Atomic structure coordinates for a representative structure of the LBD of ROR $\alpha$  in complex with cholesterol-sulfate (numbering according to Swissprot P35398-2).

Figure 1: Sequence of human ROR $\alpha$  (Swissprot P35398-1).

Figure 2 shows a schematic representation of the X-ray structure of the complex between ROR $\alpha$ -LBD and cholesterol.

Figure 3 shows a zoomed in view of the complex between ROR $\alpha$ -LBD and cholesterol (numbering according to Swissprot P35398-1).

Figure 4: Proposal of ligands in order to increase the affinity and to obtain antagonistic activity (numbering according to Swissprot P35398-1)..

Figure 5: Proposal of further derivatives of cholesterol in order to increase the affinity (numbering according to Swissprot P35398-1)..

Figure 6 shows the displacement of cholesterol by 25-OH cholesterol and cholesterol sulfate.

Figure 7 shows a zoomed view of X-ray structure of ROR(alpha)/cholesterol (numbering according to Swissprot P35398-2)..

Figure 8 Overview of interactions made by cholesterol-sulfate with LBP of ROR(alpha) (numbering according to Swissprot P35398-2)..

Figure 9 Comparison of the X-ray structures of ROR(alpha)/cholesterol-sulfate and ROR(alpha)/cholesterol (numbering according to Swissprot P35398-2).

Figure 10 Comparison of the X-ray structures of ROR(alpha)/cholesterol (left) and ROR(alpha)/cholesterol-sulfate (right) (numbering according to Swissprot P35398-2).

Figure 11 Sequence of the construct used in crystallization. The secondary structure elements are shown below the sequence. Amino acids that have a nonhydrogen atom closer than 4Å to cholesterol are highlighted in red (numbering according to Swissprot P35398-2).

#### DETAILED DESCRIPTION OF THE INVENTION

The present invention provides crystals of the LBD of ROR $\alpha$ . Moreover, the present invention provides the structural determination of such crystals by X-ray crystallography. In one embodiment, the structure of the crystal has been solved to a resolution of 1.88Å. Surprisingly, it was found that the crystal contained a ligand associated to ROR $\alpha$ . The ligand was identified as cholest-5-en-3 $\beta$ -ol (cholesterol). Thus the present invention not only provides information on the spatial organization of the LBD of ROR $\alpha$  useful for instance for in-silico screening, docking and rational drug design, but also cholesterol as a ligand binding to the ROR $\alpha$  which is useful for the identification of amino acids involved in the ligand binding. The information provided in accordance with the present invention can be used as basis for the design of compounds binding to the LBD of ROR $\alpha$ , as exemplified below. The crystal LBD of ROR $\alpha$  provided by this invention can take any crystalline form, but is preferably a single crystal. In a more preferred embodiment the crystal comprises a unit cell having the

of  $a=55 \text{ \AA} \pm 5 \text{ \AA}$ ,  $b=50 \text{ \AA} \pm 5 \text{ \AA}$ ,  $c=60 \text{ \AA} \pm 6 \text{ \AA}$  and  $\beta=98.5^\circ \pm 9^\circ$  and space group  $P2_1$ . Preferably, the unit cell dimensions are  $a=55.9 \text{ \AA} \pm 2 \text{ \AA}$ ,  $b=49.9 \text{ \AA} \pm 2 \text{ \AA}$ ,  $c=60.7 \text{ \AA} \pm 2 \text{ \AA}$  and  $\beta=98.7^\circ \pm 5^\circ$  or  $a=54.4 \text{ \AA} \pm 2 \text{ \AA}$ ,  $b=49.9 \text{ \AA} \pm 2 \text{ \AA}$ ,  $c=60.7 \text{ \AA} \pm 2 \text{ \AA}$ ,  $\beta=97.8^\circ \pm 5^\circ$ . In another preferred embodiment, the crystalline LBD of ROR $\alpha$  is of human origin. The crystalline LBD of ROR $\alpha$  according to the present invention is preferably associated with a second chemical substance. Such a substance may be any natural or synthetic chemical molecule, preferred are small molecules, more preferred are small lipophilic molecules. Cholesterol has been identified, in accordance with the present invention, as a ligand fitting into this binding pocket. Thus, in a particularly preferred embodiment such a substance is cholesterol or a cholesterol derivative. As used herein, the term "small molecule" refers to a natural or synthetic compound, preferably an organic molecule, with a molecular weight less than 3000 Da, more preferably less than 1000 Da, most preferably less than 500 Da. The term "lipophilic", as used herein, refers to compounds that are mainly unpolar and that are not or only slightly soluble in water. Typical examples may include fatty acids, retinoic acids, melatonin, steroid hormones, vitamin D derivatives. Other examples may include lipophilic molecules like tamoxifen or raloxifen. In accordance with the present invention, a particularly preferred lipophilic ligand is cholesterol and derivatives thereof. As used herein the term "cholesterol derivative" means a molecule that possesses similarity to cholesterol, such as the same overall structure, but with different substituents or differences in the location of unsaturated bonds or sterical isomers. Examples for such cholesterol derivatives can for instance be found in <http://www.steraloids.com>.

Crystals of the LBD of ROR $\alpha$  and, optionally a second chemical species can be grown by a number of techniques including batch crystallization, vapor diffusion (either by sitting drop or hanging drop) and by microdialysis. Seeding of the crystals in some instances is required to obtain X-ray quality crystals. Standard micro and/or macro seeding of crystals may therefore be used. An initial crystal can be allowed to grow over several weeks at  $4^\circ \text{ C}$  or at room temperature (ca.  $20^\circ \text{ C}$ ) from a hanging drop. Crystals then can be subsequently grown by macroseeding from the initial crystal. Once a crystal of the present invention is grown, X-ray diffraction data can be collected. A MAR imaging plate detector for X-ray diffraction data collection can be used for example. Crystals can be characterized by using X-rays produced in a conventional source (such as a sealed tube or a rotating anode) or using a synchrotron source.

Methods of characterization and data collection include, but are not limited to, precession photography, oscillation/rotation data collection and diffractometer data collection. As exemplified below, heavy atom derivatives can be obtained by soaking crystals in solution with 4 mM methylmercuric acetate for 1 hour. Data processing and reduction can be carried out using programs

(DENZO, and SCALEPACK) of the HKL-suite [Otwinowski and Minor, *Meth. Enzymol.* 276:307-326 (1997)]. Heavy atom positions can be found using programs such as SnB [Weeks, C.M. & Miller, R. (1999) *J.Appl.Cryst.* 32, 120-124.] or programs (e.g. SHELX and RSPS) of the CCP4 program suite [Collaborative Computational Project, Number4, *Acta Cryst. D*53: 760-763 (1994)]. Electron density maps can be calculated using programs (e.g. MLPHARE and DM) of the CCP4 program suite [Collaborative Computational Project, Number4, *Acta Cryst. D*53: 760-763 (1994)] or alternatively using SHARP [La Fortelle, E. D. and Bricogne, G., *Methods in Enzymology* 276:472-494 1997)] and SOLOMON. Molecular models can be built into this map using O [Jones, T. a. et al., *ACTA Crystallogr. A*47:110-119 (1991)]. A complete molecular model for the protein can be built on the basis of the experimental electron density map. Model building interspersed with positional and simulated annealing refinement using X-PLOR, [Brunger, X-PLOR v.3.1 Manual, New Haven: Yale University, (1993)] or with CNS, using a maximum likelihood residual [Brunger, A. T. et al., *Acta Cryst. D*54: 905-921 (1998)] can permit an unambiguous trace and sequence assignment of the LBD of ROR $\alpha$ .

Accordingly, the present invention provides for a model of the structure of the LBD of ROR $\alpha$  useful for rational drug design comprising a set of co-ordinates embodying the structure of the LBD of ROR $\alpha$ . Thus, a preferred embodiment provides for a model embodying the structure of the LBD ROR $\alpha$  comprising one or more sets of atomic coordinates in Table 8 or 9. Other preferred embodiments provide a computer system comprising computer hardware or the model of the present invention and a computer readable medium comprising the model of the present invention. The set of co-ordinates is preferably determined by crystallographic analysis of the LBD of ROR $\alpha$ , however any available method may be used to construct such a model using data disclosed herein or obtained from independent crystallographic analysis of the LBD of ROR $\alpha$ . The term "structure co-ordinates" refers to Cartesian co-ordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a protein or protein-ligand complex in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are then used to establish the positions of the individual atoms of the enzyme or enzyme complex. Variations in co-ordinates may be generated because of mathematical manipulations of the structure co-ordinates. For example, the structure co-ordinates set forth in Table 8 or 9 could be manipulated by crystallographic permutations of the structure co-ordinates, fractionalization of the structure co-ordinates, integer additions or subtractions to sets of the structure co-ordinates, inversion of the structure co-ordinates or any

combination of the above. Alternatively, modifications in the crystal structure due to mutations, additions, substitutions, and/or deletions of amino acids, or other changes in any of the components that make up the crystal could also account for variations in structure co-ordinates. If such variations are within an acceptable standard error as compared to the original co-ordinates, the resulting three-dimensional shape is considered to be the same. Various computational analyses are therefore necessary to determine whether a molecule or molecular complex or a portion thereof is sufficiently similar to all or parts of the structure of the LBD of ROR $\alpha$  as to be considered the same. Such analyses may be carried out in current software applications, such as the Molecular Similarity application of QUANTA (Molecular Simulations Inc., San Diego, Calif.) version 4.1, and as described in the accompanying User's Guide. For the purpose of this invention, any molecule or molecular complex that has a root mean square deviation of conserved residue backbone atoms (N, C $\alpha$ , C, O) of less than 1.5 Å; when superimposed on the relevant backbone atoms described by structure co-ordinates listed in Table 8 or 9 are considered identical. More preferably, the root mean square deviation is less than 1.0 Å. The term "root mean square deviation" means the square root of the arithmetic mean of the squares of the deviations from the mean. It is a way to express the deviation or variation from a trend or object. For purposes of this invention, the "root mean square deviation" defines the variation in the backbone of a protein or protein ligand complex from the relevant portion of the backbone of the LBD of ROR $\alpha$  as defined by the structure co-ordinates described herein.

In certain embodiments, the data set embodies a portion of the structure of the LBD of ROR $\alpha$ , including without limitation the binding pocket of LBD of ROR $\alpha$ . The term "binding pocket", as used herein, refers to a region of a molecule or molecular complex, that, as a result of its shape, favorably associates with another chemical entity or compound. In accordance with the present invention, a preferred binding pocket includes the amino acids shown in Figures 3, 4, 5, 7, 8, 9 or 10 one or more of the following amino acids: Cys321, Gln322, Tyr323, Leu328, Trp353, Cys356, Ala357, Lys359, Ile360, Glu362, Ala363, Val397, Phe398, Arg400, Met401, Arg403, Ala404, Val412, Tyr413, Phe414, Phe424, Leu427, Cys429, Phe432, Ile433, Val436, His517, Lys520 and Tyr540 (numbering according to SWISS-PROT P35398-1).

In one embodiment of the present invention, the model may be used to identify substances that interact with the LBD of ROR $\alpha$ . In general, molecular similarity applications in accordance with the present invention permit comparisons between different structures, different conformations of the

same structure, and different parts of the same structure. A potential interacting substance is examined through the use of computer modeling using a docking program such as GRAM, DOCK, or AUTODOCK [Dunbrack et al., *Folding & Design*, 2:27-42 (1997)]. This procedure can include computer fitting of potential ligands to the LBD of ROR $\alpha$ , for example to ascertain how well the shape and the chemical structure of the potential ligand will complement with the binding pocket provided by the present application. Computer programs can also be employed to estimate the attraction, repulsion, and steric hindrance of the ligand to the LBD of ROR $\alpha$ . Generally the tighter the fit (e.g., the lower the steric hindrance, and/or the greater the attractive force) the more potent the potential drug will be since these properties are consistent with a tighter binding constant. Furthermore, the more specificity in the design of a potential drug the more likely that the drug will not interfere with other properties of the ROR $\alpha$  protein or other proteins (particularly proteins present in the nucleus). This will minimize potential side-effects due to unwanted interactions with other proteins. Initially a potential interacting substance could be obtained by screening a chemical library. A ligand selected in this manner could then be systematically modified by computer modeling programs until one or more promising potential ligands are identified. Alternatively, a known ligand of ROR $\alpha$ , such as for instance cholesterol as identified in accordance with this invention, may be used as a starting point for systematic modification. Such computer modeling allows the selection of a finite number of rational chemical modifications, as opposed to the countless number of essentially random chemical modifications that could be made, and of which any one might lead to a useful drug. Each chemical modification requires additional chemical steps, which while being reasonable for the synthesis of a finite number of compounds, quickly becomes overwhelming if all possible modifications needed to be synthesized. Thus through the use of the three-dimensional structures disclosed herein and computer modeling, a large number of these compounds can be rapidly screened on the computer monitor screen, and a few likely candidates can be determined without the laborious synthesis of untold numbers of compounds.

Accordingly, methods for identifying substances that bind to the LBD of ROR $\alpha$  are provided. Such methods typically include the steps of providing a model embodying the structure of the LBD of ROR $\alpha$ , assessing the interaction of a candidate substance with said model, selecting a substance which is predicted to interact with the LBD of ROR $\alpha$ , and, optionally, contacting the selected substance with the LBD of ROR $\alpha$ . In a preferred embodiment, such a method includes comparing the 3-D structure of candidate compounds with the 3-D molecular model shown in Table 8 or 9 or with the co-ordinates of amino acids which are part of a preferred binding pocket or directly or indirectly involved in binding of a ligand, as herein disclosed for instance in Figures 3, 4, 5, 7, 8, 9 or 10.

Preferably, said amino acids can form hydrogen bonds with hydrogen bonding functional groups (directly or via water molecules) in a candidate compound or can form favorable vdW-interactions. The interactions are preferably assessed by a computer-assisted method, such as for instance a data processing method in which the structure co-ordinate data as described above is input in a data structure such that the interatomic distances between the atoms of the LBD of ROR $\alpha$  are easily retrieved, and the distances between hydrogen-bonding functional groups of different candidate compounds and hydrogen bonding atoms of the amino acids that form the binding pocket in the 3D molecular model are compared (or the distances between groups forming vdW-interactions) thereby allowing the identification of those candidate compounds which would theoretically form the most stable complexes with the 3-D molecular model binding pocket of the LBD of ROR $\alpha$ , based on optimal hydrogen bonding and vdW-interactions between the two structures.

In a preferred embodiment the substances are designed to interact via vdW-interactions or via hydrogen bond interactions directly or indirectly (e.g. via water molecules) with atoms of one or more amino acids shown in Figures 3, 4, 5, 7, 8, 9 or 10 or selected from the group consisting of Cys321, Gln322, Tyr323, Leu328, Trp353, Cys356, Ala357, Lys359, Ile360, Glu362, Ala363, Val397, Phe398, Arg400, Met401, Arg403, Ala404, Val412, Tyr413, Phe414, Phe424, Leu427, Cys429, Phe432, Ile433, Val436, His517, Lys520 and Tyr540, Gln322, Tyr323, Arg400, Arg403. In a more preferred embodiment the substances interact via vdW-interactions or via hydrogen bond interactions directly or indirectly (e.g. via water molecules) with atoms of one or more amino acids selected from the group consisting of Gln322, Tyr323, Arg400, Arg403 or Trp353, Lys359, Ile360, Ala363, Met401, Phe414, Leu427, Phe432, Val436. Substances identified using the above methods are also provided. Preferred substances are small molecules, more preferred are small lipophilic molecules (possibly with a polar group) and particularly preferred are cholesterol or cholesterol derivatives, such as for instance cholesterol sulfate. In a further preferred embodiment, the binding constant of the substance to ROR $\alpha$  is at least 1 $\mu$ M, preferably at least 100nM, more preferably at least 10nM.

In addition, agonists and antagonists of ROR $\alpha$  are provided. In one embodiment methods for screening for agonists or antagonists of ROR $\alpha$  are provided. Such methods include selecting a potential agonistic or antagonistic compound by performing rational drug design with one or more sets of atomic co-ordinates embodying the structure of the LBD of ROR $\alpha$ , contacting the potential compound with a LBD of ROR $\alpha$  and measuring the biological activity of ROR $\alpha$ . The selection is typically made in conjunction with computer modeling. A potential compound is identified as agonist if it increases the biological activity of ROR $\alpha$  or as antagonist if it decreases the biological activity of



ROR $\alpha$ . Agonists and antagonists identified by such methods are also provided. The agonist or antagonist needs not to bind to the binding pocket used by the natural ligand of ROR $\alpha$ , but could also bind at another position and exert its effect allosterically. A preferred embodiment of an agonist according to the present invention is a compound that stabilizes helix 12 (H12) in the agonistic position, i.e. the position in which H12, together with the H3–H4 region, forms the proper interaction surface, i.e. the complete AF-2, for the coactivator (reviewed e.g. in Renaud & Moras, Cell. Mol. Life Sci., 57, 1748–1769, 2000). A preferred embodiment of an antagonist according to the present invention is a compound that destabilizes the agonistic position of H12 for instance by tilting the position of H12 (reviewed e.g. in Renaud & Moras, 2000, *supra*). Destabilisation of H12 may for instance be achieved by a cholesterol derivative with a bulky substituent at position 26 thus displacing Tyr540 and / or His517. In a preferred embodiment such agonists or antagonists are small molecules. Particularly preferred are lipophilic small molecules. Examples without being limiting are for instance fatty acids, retinoic acids, melatonin, steroid hormones, vitamin D derivatives, but also compounds similar to tamoxifen or raloxifen or derivatives thereof. In one embodiment, such agonists or antagonists may be cholesterol or cholesterol derivatives. In a preferred embodiment of this invention the cholesterol ligand has been modified using the structural information provided by the present invention to a cholesterol derivative binding more strongly to the ligand binding pocket (LBP) of the LBD of ROR $\alpha$  provided by the present invention. An example for a more strongly, competitively binding cholesterol derivative that has been designed using the structural information provided by this invention is cholesterol sulfate (see below). In another preferred embodiment, the present invention provides a pharmaceutical composition comprising a therapeutically effective amount of a compound stabilizing H12 of ROR $\alpha$  in an agonistic position and a pharmaceutically acceptable carrier. In a related embodiment, the present invention provides a pharmaceutical composition comprising a therapeutically effective amount of a compound destabilizing H12 of ROR $\alpha$  in an agonistic position and a pharmaceutically acceptable carrier.

Once a potentially binding substance, such as an agonist or antagonist, is identified it can be either selected from a library of chemicals or alternatively the potential ligand may be synthesized de novo. The de novo synthesis of one or even a relatively small group of specific compounds is reasonable in the art of drug design. The prospective drug can be placed into any standard binding assay to test its effect on any particular ROR $\alpha$  function, for instance on the DNA binding of ROR $\alpha$  exemplified below. When a suitable drug is identified, a supplemental crystal can be grown which comprises a protein-ligand complex, for instance formed between the binding pocket of the LBD of ROR $\alpha$  and the

drug. Preferably the crystal effectively diffracts X-rays allowing the determination of the atomic coordinates of the protein-ligand complex to a resolution of greater than 5.0 Angstroms, more preferably greater than 3.0 Angstroms or greater than 2.0 Angstroms. The three-dimensional structure of the supplemental crystal can be determined by molecular replacement analysis. Molecular replacement involves using a known three-dimensional structure as a search model to determine the structure of a closely related molecule or protein-ligand complex in a new crystal form. The measured X-ray diffraction properties of the new crystal are compared with the search model structure to compute the position and orientation of the protein in the new crystal. Computer programs that can be used include: programs (AMORE , MOLREP) of the CCP4 program suite [Collaborative Computational Project, Number 4, Acta Cryst. D53: 760-763 (1994)] or X-PLOR [Brunger, X-PLOR v.3.1 Manual, New Haven: Yale University, (1993)]. Once the position and orientation are known an electron density map can be calculated using the search model to provide X-ray phases. Thereafter, the electron density is inspected for structural differences and the search model is modified to conform to the new structure. Using this approach, it will be possible to use the claimed structure to solve the three-dimensional structures of any such LBD of ROR $\alpha$  complex. For all of the drug screening assays described herein further refinements to the structure of the drug will generally be necessary and can be made by the successive iterations of any and/or all of the steps provided by the particular drug screening assay.

The substances identified by rational design can be further analyzed in drug screening assay. The drug screening assays of the present invention may use any of a number of assays for measuring the functionality of ROR $\alpha$ , including for the ability of ROR $\alpha$  following ligand binding to transcriptionally regulate a gene, by increasing phosphorylation of ROR $\alpha$ , by allowing ROR $\alpha$  to dimerize or to heterodimerize with another nuclear receptor, by improving its ability to interact with co-activators, by changing its conformation and by increasing its ability to bind DNA. In one binding assay, a nucleic acid containing a ROR $\alpha$  binding site is placed on a coated or onto a solid support. A preferred binding site is a response element (RORE) composed of a 6 bp AT rich motif immediately preceding a half site AGGTCA and the possible variants of this response element that are given in Giguere et al. 1994, Genes & Development 8:538-553, Mc Broom et al. 1995 Mol. Cell. Biol. 15: 796 - 808, Moraitis & Giguere, 1999; Molecular Endocrinology. 13:431-439. Methods for placing the nucleic acid on the solid support are well known in the art and include linking biotin to the nucleic acid and linking avidin to the solid support. The ROR $\alpha$  is allowed to equilibrate with the nucleic acid and drugs are tested to see if they disrupt or enhance the binding.

In another assay, a co-activator protein, such as for instance GRIP or DRIP 205 (Brandon-Atkins et al. 1999, *Molecular Endocrinology* 13: 1550-1557), or SRC1, NcoA-1, ERAP / P160, SRC2 / NcoA-2, ACTR, SRC-3, pCIP, ERAP -140, RIP 140, RIP 160 P/Caf, CBP/P), ARA70 , Ada 3, Rap 46, GRIP170, TRIP 1, PGC1 and 2, SPT6, TIF $\alpha$ , SW1/SNUERF, TRAP 100, TRAP 220, DRIP, NSD1 (Robyr et al. 2000, *Mol. Endo.* 14: 329-347), are placed on a coated or onto a solid support. The ROR $\alpha$  protein may be labeled. For example, in one embodiment radiolabeled ROR $\alpha$  proteins are used to measure the effect of a drug on binding. In another embodiment the natural ultraviolet absorbance of the ROR $\alpha$  protein is used. In yet another embodiment, a Biacore chip (Pharmacia) coated with the co-activator peptide is used and the change in surface conductivity can be measured. In yet another embodiment, the effect of a prospective drug (a candidate compound) on interactions between ROR $\alpha$  and their DNA binding sites are assayed in living cells that contain or can be induced to contain activated ROR $\alpha$  proteins. Cells containing a reporter gene, such as the heterologous gene for luciferase, green fluorescent protein, chloramphenicol acetyl transferase or  $\beta$ -galactosidase and the like are operably linked to a promoter containing a ROR $\alpha$  binding site. A prospective drug is then contacted with the cell. The amount (and/or activity) of reporter produced in the absence and presence of prospective drug is determined and compared. Prospective drugs which reduce the amount (and/or activity) of reporter produced are candidate antagonists of the ROR $\alpha$  DNA binding, whereas prospective drugs which increase the amount (and/or activity) of reporter produced are candidate agonists of ROR $\alpha$  DNA binding. Assays for detecting the reporter gene products are readily available in the literature. For example, luciferase assays can be performed according to the manufacturer's protocol (Promega), and beta-galactosidase assays can be performed as described by Ausubel et al., [in *Current Protocols in Molecular Biology*, J. Wiley & Sons, Inc. (1994)]. In one example, the transfection reaction can comprise the transfection of a cell with a plasmid modified to contain a ROR $\alpha$  protein.

In one embodiment, the prospective drugs identified by the methods of this invention can be tested for pharmacological activity using assays known in the art. For example, the identified prospective drugs can be tested for activity as potential drugs for the prophylaxis or treatment of a disease or medical condition which involves excessive bone or cartilage loss using a method as disclosed in WO 01/26737. For instance, a reporter assay can be carried out using the bone sialoprotein (BSP) or osteocalcin (OC), which are known modulators of bone mineralization and remodelling. Suitable cells can be transfected with a reporter construct in which a BSP or an OC promoter drive a reporter gene, such as the firefly luciferase gene. A prospective drug is then contacted with the cell. The amount of

luciferase activity produced in the absence and presence of prospective drug is determined and compared. In another embodiment, the system for testing prospective drugs according to the present invention can be the use of classical ovariectomized rat model, the loss of ovarian function induces a drop in circulating estrogen promptly followed by decrease of bone mass (Wronski et al., *Calcified Tissue International*. 45(6):360, 1989). The drug will be tested on ovariectomized animal for a curative treatment of 8 weeks started twelve weeks after ovariectomy and bone mineral density will be monitored. Another type of experiment could be envisaged which is a preventive treatment of intact animals for eight weeks.

Cholesterol has been found to be a ligand of ROR $\alpha$ . In accordance with this finding, the present invention provides novel assay methods for the identification of compounds binding to ROR $\alpha$ , in particular for the identification of compounds modulating ROR $\alpha$  activity, wherein interactions between the candidate compounds and ROR $\alpha$  are allowed to take place in a surrounding reduced in cholesterol, preferably free of cholesterol. Such a method typically includes the steps of (a) contacting ROR $\alpha$  with a candidate compound, (b) measuring interactions between the candidate compound and ROR $\alpha$  in a surrounding essentially free of cholesterol, and (c) selecting said compound if it interacts with ROR $\alpha$ . Though not a requirement, it is preferred that all method-steps are carried out in the cholesterol-reduced, or preferably essentially cholesterol-free, surrounding. In a more preferred embodiment, such a method relates to a eukaryotic cellular system. In a yet even more preferred embodiment insect cells are used. Insect cells differ from eukaryotic cells by lacking the capacity for de novo sterol synthesis. It has been shown that these cells can be propagated under cholesterol-free conditions (Cleverley et al. 1997, *Exp. Cell Res.* 233: 288-296). Thus, such a cell system could for instance provide an appropriate cell background to monitor the activity of a ROR $\alpha$  ligand using the ROR $\alpha$  cloned in an appropriate insect cell vector and the classical reporter ROREtkluc. In another embodiment, eukaryotic cells, preferably human cells, are used. These cells can for instance be cultured in medium essentially free of cholesterol and in serum essentially free of LDL- cholesterol (the LDL - free serum preparation is described in Goldstein et al 1983, *Methods in Enzymology* 98:241-260). Mammalian cells are able to produce cholesterol endogenously. The meaning of essentially cholesterol-free surrounding according to the present invention does not include such endogenously produced cholesterol. In a particular embodiment, endogenously cholesterol producing mammalian cells could for instance be used in an assay to screen the ability of a compound to displace endogenous cholesterol.

Nuclear receptors are known to regulate the transcription of specific genes or sets of genes upon ligand binding, which makes them interesting targets for the screening for compounds useful as therapeutics. So far, however, deeper understanding of the molecular mechanism of ROR $\alpha$  that could lead to development of therapeutics has been severely hampered by the lack of knowledge of a ligand that binds the LBD of ROR $\alpha$ . The identification of cholesterol as ligand of the receptor ROR $\alpha$  in accordance with the present invention, now provides new insights into the physiological role of ROR $\alpha$  and provides ROR $\alpha$  as a target for the screening for compounds useful for the treatment of cholesterol related-diseases. It has been shown that defects in cholesterol biosynthesis lead to a variety of clinical characteristics (Nwokoro et al., Mol Genet Metab 74:1-2 105-19 2001), covering brain damage, skeletal defects, with in some cases osteosclerosis, limb aplasia or vertebral hypoplasia. Thus, cholesterol related diseases may include endocrine disorders, atherosclerosis and cardiovascular diseases, metabolic diseases such as for instance obesity, inflammatory diseases, skin diseases, diseases related to the CNS, such as for instance Alzheimer disease and disorders in cell proliferation and apoptosis such as tumor related diseases.

In one embodiment, the present invention provides ROR $\alpha$  as target for the screening of compounds useful for the treatment of endocrine disorders, in particular disorders that are related to the synthesis of steroid hormones or the regulation of steroidogenesis. In all steroidogenic tissues, regardless of the hormones synthesized, the initial step in steroidogenic cells is the conversion of cholesterol to the first steroid, pregnenolone (Stocco, Ann Rev Physiol 63: 193-213; 2001).

In another embodiment, the present invention provides ROR $\alpha$  as target for the screening of compounds useful for the treatment of disorders of the cholesterol homeostasis. Breakdown of cholesterol homeostasis causes disease states, the most common being atherosclerosis. Hypercholesterolemia is a well-known risk factor. Using statins the present inventions shows a direct link between the activity of ROR $\alpha$  and a potent anti-atherosclerosis molecule (Table 5) demonstrating the usefulness of ROR $\alpha$  as molecular target for the search of compounds to fight atherosclerosis and cardiovascular diseases.

In another embodiment, the present invention provides ROR $\alpha$  as target for the screening of compounds useful for the treatment of metabolic disorders. It is known that a cascade of events initiates adipogenesis where C/EBP and PPAR $\gamma$  are important players. Furthermore, ROR $\alpha$  is able to strongly induce PPAR $\gamma$  (Sundvold et al. Biochem. Biophys. Res. Com. 287: 383-390; 2001). SREBP

promotes the adipogenic program and SREBP activity is sensitive to the level of intracellular cholesterol (Brown et al. Cell 89: 331-340,1997). Thus, in accordance with this invention, ROR $\alpha$  is provided as a target for the screening of compounds useful for the treatment of disorders related to adipogenesis, development of obesity and insulin resistance, which can lead to type 2 diabetes. Furthermore, the mature adipocytes secrete factors that play a role in immunological responses, vascular disease and appetite regulation. Adipocytes derived factors include leptin, prostaglandin's and resistin. The present invention providing cholesterol as ligand of ROR $\alpha$  thus provide ROR $\alpha$  as target for screening for compounds useful for the treatment of diseases related to immune response, vascular disease and appetite regulation.

It has recently been shown that mesenchymal stem cells have the potential to differentiate into these three lineage (Pittenger et al., 1999 Science 284:143-147). Thus, an apparent reciprocal relationship is postulated to exist between the adipocyte and osteoblast phenotypes. This balance is switched toward adipocytes in osteoporotic patients. This invention provides ROR $\alpha$  (as PPAR $\gamma$  or C/EBP) as important players in the adipogenesis pathway or in the differentiation of mesenchymal stem cells into adipocytic, chondrocytic or osteoblastic lineage. Thus, the present invention links ROR $\alpha$  in this switch toward adipogenesis and therefore is a potential target for therapeutic intervention in osteoporosis.

In another embodiment, the present invention provides ROR $\alpha$  as target for the screening of compounds useful for the treatment of inflammatory diseases. Molecular links have been established between cholesterol and cytokines showing the involvement of inflammation and immunity in atherogenesis. In addition, ROR $\alpha$  is involved in inflammation (WO01/26737, Bourdji et al. J. Biol Chem.275: 12243-12250 2000, Delerive et al., EMBO reports 21: 42-48; 2001).

In another embodiment, the present invention provides ROR $\alpha$  as target for the screening of compounds useful for the treatment of skin disorders. ROR $\alpha$  is highly expressed in skin (Becker-Andre, 1993; Biochem. Biophys. Res. Commun. 194:1371-1379). In addition, clinical observation of patients with genetic disorders of cholesterol biosynthesis report photosensitivity and patchy alopecia, as well as follicular atrophoderma.

In another embodiment, the present invention provides ROR $\alpha$  as target for the screening of compounds useful for the treatment of Alzheimer disease. The lipoprotein allele ApoE4 is associated with an increased incidence of Alzheimer disease (Trittmatter et al. Proc. Natl. Acad. Sci.USA 90:

1977-1981; 1993); the depletion of plasma membrane cholesterol in hippocampal neurons inhibits the formation of Abeta (Simons et al. PNAS 95: 6460-6464;1998), the cleavage product of the amyloid precursor protein, that is a key factor in the pathogenesis of the disease. In addition the main characteristics of the ROR $\alpha$  knock out mice is a severe ataxia and their cerebellum is markedly atrophied. This is implicated in rare inherited disease where people are subject to movement disorders.

## EXAMPLES

### Cloning and expression of (His)<sub>6</sub>ROR $\alpha$ -LBD304-556

A DNA fragment encoding part of polyhedrin promoter up to the ATG codon is amplified by PCR from the pBAKPac8 plasmid (Clontech) by using the oligonucleotide RS365 (5'-ACCATCTCGCAAATAAATAAG-3') and MG384 (5'-ATGATGATGATGATGATGGC-TGCTGCCCATGGTGGGAACCTCGAGGCCTGCAGGG-3'). MG384 has a 5' extension not present on the template DNA but which is encoding for a Kozak sequence in front of the ATG codon and part of the His tag which will be present in the final engineered vector. The second PCR reaction is run with the oligonucleotides MG383 (5'-GCCATCATCATCATCATC-ATCTGGAAGTTCTGTTCCAGGGGCCCCGAGAATTAGAACACCTTGC-3') and MG385 (5'-GTACCAGATCTTCTAGATTTCGTTACCCATCAATTTGCATTG-3') on a plasmid template encoding the ligand binding domain (aa304 to aa 556; numbering according to SWISS-PROT P35398-1) of the ROR $\alpha$  protein. As for the first PCR fragment, the oligonucleotide MG383 has a 5' extension complementing the extension present on the first PCR fragment and which is added by the extension of the fragment by MG384. By mixing both new fragments and with an PCR amplification with MG365 and RS365 a new fragment encoding the Kozak sequence, the ATG, the (His)<sub>6</sub>-tag and the cleavage site for the PreScission protease cleavage site (AmershamPharmacia) is introduced in front of the ROR $\alpha$  ligand binding domain. This new fragment has at the both end two homology regions in common with the target plasmid pBAKPac8. The integration of the engineered gene into the cloning vector is done by using the method we described earlier (Geiser et al, BioTechniques 31 88-92 ,2001). DNA sequence analysis of the resulting clones confirms that the clone is as intended. The plasmid is called pXI338.

The plasmid pXI338 is co-transfected with linearised BacPAK6 (AcNPV) virus DNA into Sf-21 insect cells using lipofection. The viral supernatant harvested after five days is subjected to plaque purification to obtain homogenous virus populations, which are subsequently amplified on small scale and analyzed for production by Western blotting. A band of correct size is readily detectable using an

anti-ROR $\alpha$  antibody (Santa Cruz, Cat.No. sc-6062) in all six analyzed cell pellets. One viral isolate is chosen for further amplification; a master virus stock, followed by a working virus stock are generated by further amplification in Sf-9 cells; titers are determined by plaque assay. A kinetic experiment reveals optimal production conditions for ROR $\alpha$ -sLBD using 1 MOI at  $1.82 \times 10^6$  cells/ml (TOI) for 72 hours. Under these conditions a large fraction of the protein remained soluble in the insect cells. Two Wave Bioreactor runs are performed of approx. 10-13 liters each under the above described conditions. Cells are harvested by centrifugation for 10 minutes at 6000 g in a Heraeus Cryofuge M7000, and the pellets are stored at -80° C.

#### Purification and characterization of (His)<sub>6</sub>ROR $\alpha$ -LBD<sub>304-556</sub>

(His)<sub>6</sub>ROR $\alpha$ -LBD<sub>304-556</sub> is purified by Ni-NTA chromatography followed by anion-exchange and size exclusion chromatography according to standard methods. From 20-g cell paste, around 15 mg of (His)<sub>6</sub>ROR $\alpha$ -LBD<sub>304-556</sub> is purified. The protein runs as a monomer on the size exclusion chromatography. N-terminal sequence analysis shows that the N-terminus is blocked. Mass spectrometry analysis shows a homogeneous molecular mass of 31'515.4 corresponding to Acetyl-desMet-(His)<sub>6</sub>ROR $\alpha$ -LBD<sub>304-556</sub> (Acet- GSSHHHHHHLEVLFGPAELEH...MQIDG). Proteolytic cleavage of the N-terminal 6xHis tag by the PreScission™ protease results in a homogeneous protein that however does not yield useful crystals. In contrast, uncleaved ROR $\alpha$ -LBD leads to crystals suitable for X-ray diffraction analysis.

#### Crystallization

Recombinant human ROR $\alpha$ -LBD in 50 mM Tris-HCl pH 7.5, 100 mM NaCl, 5 mM DTT is concentrated to 14 mg/ml. Crystallization is performed using a standard vapor diffusion hanging drop set-up, with VDX crystallization plates and siliconized microscope cover slips from Hampton Research. Crystallization droplets are made by mixing on the coverslips 2.0 $\mu$ l of the protein stock solution with 2.0 $\mu$ l of reservoir solution and equilibrated against 700 $\mu$ l of reservoir solution at 20°C. Commercially available screening kits are used to find preliminary crystallization conditions. In the refined conditions, crystals grow within 2 weeks at 20°C to a size of 0.15x 0.15 x 0.3 mm with a reservoir of 100 mM Tris-HCl pH 8.4, 19% PEG 6000, 0.2M CaCl<sub>2</sub>. The space group of the native crystals is P2<sub>1</sub>, with unit cell parameters  $a = 55.9 \text{ \AA}$ ,  $b = 49.9 \text{ \AA}$ ,  $c = 60.7 \text{ \AA}$ ,  $\beta = 98.7^\circ$  and space group P2<sub>1</sub>. There is one monomer per asymmetric unit. The crystals diffract at the synchrotron (SNBL at ESRF, Grenoble) to at least 1.88  $\text{\AA}$ .



### X-ray data collection

For the native data collection, a crystal grown as described above is transferred to 5 $\mu$ l of solution containing 20% glycerol (in addition to the reservoir composition) for about 10 seconds. The crystal is then rapidly mounted in a nylon CryoLoop (Hampton Research) and directly frozen in a cold nitrogen stream for X-ray data collection at 105K. Diffraction data are collected with the mar345 image plate system of the Swiss-Norwegian beamline of the European Synchrotron Radiation Facility ( $\lambda=0.8727\text{\AA}$ ). A total of 230 images of  $1.0^\circ$  rotation each are collected in time mode (15sec per frame) with a crystal-to-detector distance of 178mm (using a readout plate-diameter of 180mm). Raw diffraction data are processed and scaled with the HKL program suite version 1.96.6 (Otwinowski and Minor, 1996). Crystal data and data collection statistics for the native data are shown in Table 4. The space group of the native crystals is  $P2_1$ , with unit cell parameters  $a = 55.9\text{\AA}$ ,  $b = 49.9\text{\AA}$ ,  $c = 60.7\text{\AA}$ ,  $\beta = 98.7^\circ$ . There is one monomer per asymmetric unit. The estimated  $B$ -factor by Wilson plot is  $30\text{\AA}^2$ . For the Hg-derivative data collection, a crystal is soaked previously for 1hr in 5 $\mu$ l of solution containing 4mM methylmercuric acetate (in addition to the reservoir composition). Cryocooling is then done as for the native crystal. Diffraction data are collected with the mar345 image plate system of the Swiss-Norwegian beamline of the European Synchrotron Radiation Facility ( $\lambda=0.8727\text{\AA}$ ). A total of 287 images of  $1.0^\circ$  rotation each are collected in time mode (15sec per frame) with a crystal-to-detector distance of 178mm (using a readout plate-diameter of 180mm). Raw diffraction data are processed and scaled with the HKL program suite version 1.96.6 (Otwinowski and Minor, 1996). Crystal data and data collection statistics for the Hg-derivative data are shown in Table 2. The space group of the Hg-derivative crystals is  $P2_1$ , with unit cell parameters  $a = 55.6\text{\AA}$ ,  $b = 50.0\text{\AA}$ ,  $c = 60.1\text{\AA}$ ,  $\beta = 98.0^\circ$ . There is one monomer per asymmetric unit. The estimated  $B$ -factor by Wilson plot is  $29\text{\AA}^2$ .

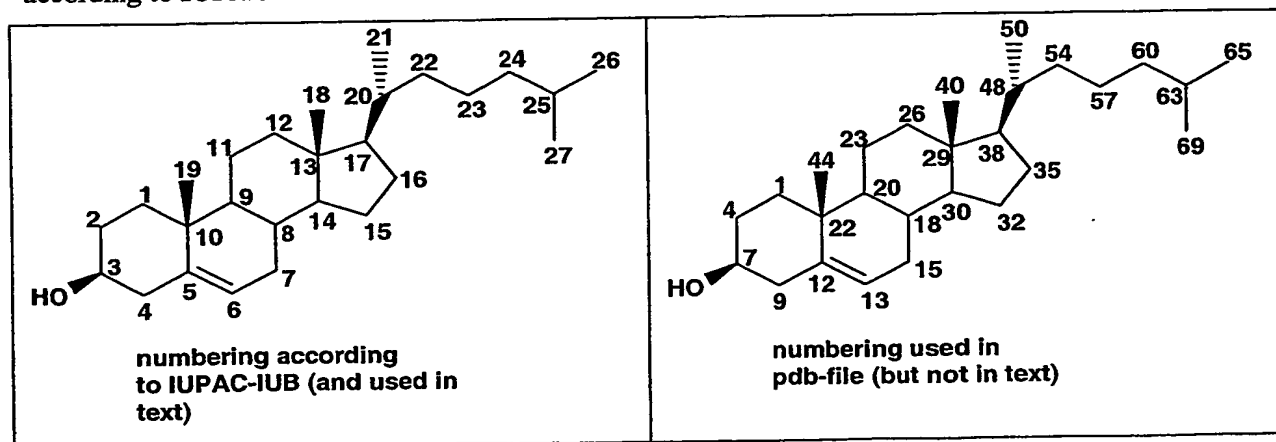
### Structure solution

Attempts to solve the structure by molecular replacement with the programs AmoRe (Navaza, 1994) or MOLREP version 6.2.5. (Vagin & Teplyakov, J.Appl.Cryst. 30, 1022-1025, 1997) by using several different models based on the coordinates of the pdb-entries 2lbd (hRAR $\gamma$ ) or 1bsx (hTR $\beta$ ) are not successful. Data from a single-wavelength experiment on the mercury-substituted crystal are thus used together with a native data set for the initial phasing by SIRAS. Anomalous as well as isomorphous difference Patterson maps reveal at least one common dominant peak. SnB version 2.1 (Weeks & Miller, J.Appl.Cryst. 32, 120-124, 1999) with DREAR normalization (Blessing & Smith, J.Appl.Cryst. 32, 664-670, 1999) using the observed anomalous differences is used to determine 4 Hg-

sites. The heavy-atom parameters are subsequently refined using MLPHARE version 4.1 (CCP4, 1994). Subsequent density modification with DM (CCP4, 1994) result in an excellent experimental SIRAS-map. Skeletonization with mapman enables chain-tracing and model building with O version 7.0 (Jones *et al.*, Acta Crystallogr. A47:110-19, 1991).

### Refinement

After building the protein (residues His308-Phe544 had visible electron density) and insertion of 112 water molecules into the experimental SIRAS-map, several alternate cycles of refinement and manual rebuilding result in a model with  $R_{\text{cryst}} = 28.1\%$  ( $8\text{\AA}$ - $1.88\text{\AA}$ ), that give excellent 2Fo-Fc and Fo-Fc maps for a ligand in the LBP. The excellent quality of the electron density allows the unambiguous identification of the ligand as being cholest-5-en-3 $\beta$ -ol (cholesterol). The cholesterol ligand is then built into the electron density and X-PLOR parameter- and structure-files can be generated with the program XPLO2D (Kleywegt G., CCP4/ESF-EACBM Newsletter on Protein Crystallography 31, 45-50, 1995) that can be used to generate the X-PLOR parameter- and structure-files. Further cycles of refinement and insertion of 119 more water molecules (leading to a total of 231 water molecules) yield the final  $R_{\text{cryst}} = 24.8\%$  and  $R_{\text{free}} = 26.3\%$  (no sigma cutoff,  $8\text{\AA}$ - $1.8\text{\AA}$ , working set of 25592 unique reflections, test set of 1279 reflections). In general, the electron density is of excellent quality, except for the loop 493-498 which has weak density (residues 308-544 are included in model). Refinement is done with X-PLOR 3.1 (A.Bruenger, X-PLOR Version 3.1: A system for X-ray Crystallography and NMR. Yale University Press, New Haven, CT, USA, 1992) using the Engh and Huber force field for the protein (Engh & Huber, Acta Crystallogr. A47:392-400, 1991). The chain identifiers used are A for the protein (residues His308-Phe544, numbering according to SWISS-PROT P35398-1), L for the ligand (cholesterol: residue 1) and V for the water molecules (total of 231). The atom numbers used for the ligand cholesterol in the pdb-file are not the same as the atom numbers according to IUPAC-IUB.



The quality of the model is assessed with X-PLOR 3.1 (A.Bruenger, id 1992) and PROCHECK v3.3 (Laskowski *et al.*, J. Appl. Cryst. 1992; 26:283-91) (see Table 3). The final model of the complex ROR $\alpha$ /cholesterol has good geometry (rms bond lengths = 0.013Å, rms bond angles = 1.46°) and no residues are in disallowed regions of the Ramachandran plot, as determined by PROCHECK v3.3. Molecular graphics pictures are made with O version 7.0 (Jones *et al.*, id 1991).

Table 1:

Number of crystals	1
Space group	P2 <sub>1</sub>
Unit cell dimensions	55.9Å, 49.9Å, 60.7Å $\beta=98.7^\circ$
Number of monomers / a.u.	1
Packing coefficient	3.2Å <sup>3</sup> /Da
Resolution range	15.0 – 1.88Å
Number of observations	109,306
Number of rejected observations	373 (0.34%)
Number of unique reflections	26,882
Wavelength	0.8727Å
Overall	
Data redundancy	4.1
Data completeness	99.2%
< I/ $\sigma$ (I) >	29.5
R <sub>sym</sub> (I)	0.056
Reflections with I $\geq$ 3 $\sigma$ (I)	75.1%
Highest resolution shell	
Resolution range	1.95-1.88Å
Completeness for shell	93.2%
R <sub>sym</sub> (I) for shell	0.437
Reflections with I $\geq$ 3 $\sigma$ (I)	30.5%

Table 2:

Number of crystals	1
Space group	P2 <sub>1</sub>
Unit cell dimensions	55.6Å, 50.0Å, 60.1Å $\beta=98.0^\circ$
Number of monomers / a.u.	1
Packing coefficient	3.2Å <sup>3</sup> /Da
Resolution range	10.0 – 1.88Å
Number of observations	121,716
Number of rejected observations	4140 (3.4%)
Number of unique reflections	25,136
Wavelength	0.8727Å

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<b>Overall</b>	
Data redundancy	4.8
Data completeness	93.6%
$\langle I / \sigma(I) \rangle$	25.3
$R_{\text{sym}}(I)$	0.057
Reflections with $I \geq 3\sigma(I)$	81.8%
<b>Highest resolution shell</b>	
Resolution range	1.95-1.88 Å
Completeness for shell	76.2%
$R_{\text{sym}}(I)$ for shell	0.354
Reflections with $I \geq 3\sigma(I)$	44.5%
<b>Resolution range used for phasing</b>	
$R_{\text{merge}}(F)$ between native and Hg	10.0-1.94 Å
No. of common reflections	23.8%
Phasing power for acentric data	23,396
Phasing power for centric data	1.16
Overall figure of merit	0.80
$R_{\text{cullis}}$ on centric zone	0.314
Heavy atom site 1 (x,y,z, occ,Bfac)	0.80
Heavy atom site 2 (x,y,z, occ,Bfac)	-0.373, -0.546, -0.754, 0.387, 23.9
Heavy atom site 3 (x,y,z, occ,Bfac)	-0.515, -0.611, -0.927, 0.429, 35.5
Heavy atom site 4 (x,y,z, occ,Bfac)	-0.839, -0.478, -0.700, 0.265, 29.3
	-0.360, -0.797, -0.896, 0.270, 36.3

Table 3:

<b>Data used in refinement</b>	
- resolution range	8.0-1.88 Å
- intensity cutoff ( $\sigma(F)$ )	0.0
- number of reflections (working set)	25,592
- number of reflections (test set)	1,279
- completeness (working +test set)	99.0%
<b>Fit to data used in refinement</b>	
- overall $R_{\text{cryst}}$	0.248
- overall $R_{\text{free}}$	0.263
<b>Number of non-hydrogen atoms</b>	
- protein atoms	1,953
- ligand atoms	28
- water molecules	231
<b>Mean B values</b>	
- mean B value for protein	38.3 Å <sup>2</sup>
- mean B value for ligand	20.1 Å <sup>2</sup>
- mean B value for water molecules	51.8 Å <sup>2</sup>
<b>Rms deviations from ideal values</b>	
- bond lengths	0.013 Å

- bond angles	1.46°
- dihedral angles	20.3°
- improper angles	1.3°
Residues in disallowed region of Ramachandran plot	0
PROCHECK G-factor	0.28

### Overall structure of the ROR $\alpha$ -LBD

The ROR $\alpha$ -LBD adopts the canonical fold for the NR-LBDs (Wurtz *et al.*, Nat Struct Biol 3, 206 1996) and in addition has the two helices H2\* and H11\*. ROR $\alpha$ -LBD is in an agonist-bound state, as judged by the position of H12 (see also Figures 2 and 3). H12 in this position, together with the H3–H4 region, forms the proper interaction surface, i.e. the complete AF-2, for the coactivator (reviewed in Renaud & Moras, Cell. Mol. Life Sci., 57, 1748–1769, 2000). No coactivator peptide is added in order to obtain this crystal structure. An additional H2\* helix is also found between H2 and H3 for the peroxisome proliferator-activated receptors (PPARs; Nolte *et al.*, Nature, 395, 137-143, 1998). H11\* is unique to ROR $\alpha$ -LBD (and ROR $\beta$ -LBD, Stehlin *et al.*, Embo J., 20, 5822–5832, 2001) among the known LBD structures; it roughly superposes with the middle part of loop 11–12 of RAR. The overall structure of ROR $\alpha$ -LBD is similar to the one of ROR $\beta$ -LBD (e.g. as judged by Fig.4 in Stehlin *et al.*, id 2001), but since the coordinates of ROR $\beta$ -LBD are not available, no quantitative comparison with ROR $\alpha$ -LBD can be made. For ROR $\alpha$ -LBD, the putative entrance site (as judged by the solvent accessible surface of the complex) for the ligand is located between H2 and H3, and not on the H12-side, as hypothesized e.g. for RAR- $\gamma$  (Renaud *et al.*, Nature, 378, 681–689, 1995). In the crystal, the ROR $\alpha$ -LBD molecule of the asymmetric unit does not form a dimer with a neighbouring molecule. This is consistent with the finding, that on native gels ROR $\alpha$ -LBD behaves as a monomer. The following Cys-residues have reacted with methylmercuric acetate (c.f. table 2 for fractional coordinates of Hg-sites): Cys321 (site 3), Cys429 (site 1), Cys505 (site 4) and Cys514 (site 2). These reactive Cys-residues are thus candidates for mutations into Ser, in order to possibly obtain soluble expression in *E. Coli*. The protein species present in the crystallization setups correspond to the following sequences His<sub>6</sub>-tag and PreScission<sup>TM</sup> cleavage site and residue 304-556 of ROR $\alpha$ -LBD: Ac-GSSHHHHHHLEVLFGQPAELEHLA...ELFTSEFEPAMQIDG

In this crystal structure, well-defined electron density is found for the subsequence residue 308-544 (numbering according to Swissprot P35398-1) .

### Identification of the ligand and description of the ligand binding pocket

A small-molecule X-ray structure of 26-OH-cholesterol from the CSD (entry FIZDUN) shows a perfect, unambiguous fit (after removal of the 26-OH group and rotation of 120° around the C24-C25 bond) into this unbiased electron density. The excellent quality of the high-resolution map thus allows the identification of the ligand as being cholest-5-en-3 $\beta$ -ol (cholesterol). A closer look on Ligand binding pocket of ROR $\alpha$  shows that C27 of the terminal isopropyl-group of cholesterol makes vdW-contacts with the sidechain of Trp353, while C26 makes vdW-contacts with the sidechain of Ile360. Substituents on C26 have the potential to influence the position of H12 (e.g. bulky substituents on C26 could displace H12 from its agonist-position, thus leading to an antagonistic derivative of cholesterol). H12 in this crystal structure adopts the agonist position. It is stabilized in the agonist position by the hydrogen bond (distance 2.8Å) between OH-Tyr540 (on H12) and NE2-His517 (on H11). These two residues are conserved among the  $\alpha$ -,  $\beta$ -, and  $\gamma$ - isotypes of ROR.

The LBP is essentially hydrophobic on the AF-2 side (H5 N-terminus, H6, H7, H10, H12) with the exception of Tyr540 and His517 which form an intermolecular hydrogen bond (distance between OH-Tyr540 and NE2-His517 is 2.8Å). The LBP is more polar on the H3 side (loop 1-2, H3, H5 C-terminus). The main chain NHs of Gln322 and Tyr323 on loop 1-2 and the side chains of Arg400 and Arg403 on H5 contribute to the generation of a positive electrostatic potential. A negatively charged substituent (e.g. SO<sub>4</sub><sup>-</sup>) on the 3-ol group could thus yield a derivative with considerably increased affinity (Figure 4). There are 12 well-ordered water molecules in the hydrophilic part. 5 of these water molecules are amongst the 7 water molecules (of the total of 231 water molecules) which have the lowest B-factors (14 Å<sup>2</sup>-24 Å<sup>2</sup>). The 3-ol group of cholesterol makes, via a network of well-ordered water molecules, water-mediated hydrogen bonds to NE-Arg403, NH2-Arg403, CO-Arg400, NH1-Arg400, NH-Tyr323, OE1-Gln322 and NH-Gln322.

The average B-value for the ligand (20.1 Å<sup>2</sup>) is lower than the average B-value for the protein (38.3 Å<sup>2</sup>), consistent with the fact that excellent electron density for all non-hydrogen atoms of cholesterol is visible. Cholesterol adopts thus a well defined, single conformation in the LBP. This is in contrast with the multiple low-energy conformations described for the non-natural ligand stearic acid present in the ROR $\beta$ -LBD (Stehlin et al., id 2001). The following residues have a non-hydrogen atom closer than 4Å to the ligand cholesterol: Trp353, Cys356, Lys359, Ile360, Ala363, Val397, Arg400, Met401, Val412, Tyr413, Phe414, Phe424, Leu427, Phe432, Val436 and His517.

#### Design of cholesterol derivative binding to LBD of ROR $\alpha$

Overall, there is a very good fit of the ligand cholesterol to the LBP. Nevertheless, a comparison of the vdW-surface of the ligand with the vdW-surface of the LBP shows that there are still a few

possibilities for derivatizations of cholesterol (Figure 4 and 5), which could increase the affinity. Additional hydrogen bonds could be gained with hydroxy-groups added to position 6 (hydrogen bond via water to OE1-Glu362), position 19 (hydrogen bond to CO-Tyr413) or position 26 (hydrogen bond to OH-Tyr540 and/or NE2-His517). Considerable electrostatic interaction energy could be gained with a charged group, e.g.  $\text{SO}_4^-$ , added to position 3 (hydrogen bonds and electrostatic interactions via water molecules to NH1-Arg400, NH2-Arg403, NE-Arg403, NH-Gln322 and/or to NH-Tyr323). Additional vdW-interactions could be gained by additional methyl-groups added to position 12 (vdW-contacts to the sidechains of Phe398, Met401), position 18 (vdW-contacts to the sidechains of Val412, Phe398), position 27 (vdW-contacts to the sidechains of Trp353, Cys429, Phe432) or an additional ethyl-group added to position 21 (vdW-contacts to the sidechains of Phe424, Ile433, Val436, Phe437). Modifications in positions 4 and 6 could be utilized to modify, if necessary, the physicochemical or pharmacokinetic parameters, without considerably changing the affinity. Derivatives in position 26, with a bulky substituent, would have the potential to destabilize H12 in its agonist-position, thus conferring an antagonistic activity on the derivative.

#### Mechanism of action for cholesterol

The present X-ray structure promotes the following structural mechanism of action: Cholesterol (or possibly a cholesterol-derivative) enters the LBP from the H2,H3-side, possibly guided by the electrostatic field generated from Arg400 and Arg403. The isopropyl-end of cholesterol (or a derivative in this position) then influences the other end of the LBP, which is in contact with H12, thus regulating the binding of a coactivator to the LXXLL-binding site. A cholesterol-derivative with a bulky substituent on C26 could displace H12 from its agonist conformation, thus preventing coactivator binding, while a cholesterol derivative which further stabilizes the hydrogen bond between Tyr540 and His517 would further enforce the agonist conformation.

#### Selected mutations of ROR $\alpha$ -LBD

Using the coordinates from the ROR $\alpha$ -LBD X-ray structure a series of point mutations in the LBP are designed which should prevent binding of cholesterol and in addition a mutation is proposed which should prevent/reduce H12-stabilization via loss of the hydrogen bond between Tyr540 (on H12) and His517 (Tyr 540 -> Phe 540 mutation). The details of the mutations are included below.

clone name	mutated amino acid	Mutated nucleic acids
SDM1-1	Cys356 -> Leu356	TGT -> TTA
SDM2-3	Ala363 -> Leu363	GCT -> CTT

<b>SDM3-4</b>	Ala404 -> Gln404	GCC -> CAA
<b>SDM4-1</b>	Phe432 -> Trp432	TTT -> TGG
<b>SDM5-8</b>	His517 -> Trp517	CAT -> TGG
<b>SDM6-2</b>	Tyr540 -> Phe540	TAC -> TTC

In a transient transfection experiment, the transcriptional activity of the ROR $\alpha$  mutants is compared to their wild type counterpart: U2OS cells are transfected with the expression vector for ROR $\alpha$  (ROR) or its mutated form together with a luciferase reporter gene bearing a consensus response element for ROR $\alpha$  (RORE-tk-luc). Luciferase activity is assayed in cells from 6 well plates and related to the activity in cells transfected with the wild type ROR $\alpha$  expression plasmid. The results are normalized to the protein content. The figure shows the mean  $\pm$  SD and on the left panel the results are expressed as % of induction compared to the activity of the wild type ROR $\alpha$ . As shown in Table 4 all mutations, in the LBP (except the mutation Phe 432->Trp 432) significantly/drastically reduce the transcriptional activity of ROR $\alpha$  leading to the conclusion that indeed ROR $\alpha$  in its active form is bound to cholesterol. The sidechain of the mutated Trp432 has the possibility to adopt a conformation for which no steric clash with cholesterol in the LBP occurs, if the sidechains of Arg516 and Lys 520 also accordingly change their conformations. Since the latter two residues are on the surface and their sidechain conformations are not stabilized by interactions, this provides an explanation for the only slight loss of transcriptional activity for the Phe432 -> Trp432 mutation, in contrast to the other mutations in the LBP, for which there is no alternate side-chain conformation possible which would prevent a steric clash with cholesterol. The mutation Tyr 540 -> Phe 540 leads to a ca. 40% loss in transcriptional activity, showing that the hydrogen bond between Tyr 540 and His 517 contributes in a significant amount to the stabilization of H12 in the agonist position.

Table 4:

<b>a.a (Swisprot P35398 -1)</b>	<b>% Activity compared to WT</b>
356	33.3
363	18.18
404	8.33
432	90.9
517	10
540	54.54

#### Effects of fluvastatin, an inhibitor of HMG CoA-reductase, on ROR $\alpha$ transcriptional activity

Mammalian cells receive cholesterol by uptake from lipoproteins (LDL - cholesterol) and are able to synthesize cholesterol through the mevalonate pathway. In a situation where cells are cultured under



conditions essentially sterol free, a key transcription factor, SREBP will be proteolytically cleaved and this releases a transcription factor to the nucleus. This transcription factor is able to transcriptionally activate HMG - CoA reductase, which is a critical step in the cholesterol biosynthesis through the mevalonate pathway. Statins, which are known drugs for hypercholesterol state are specific inhibitors of the HMG - CoA reductase. When cells are cultivated in sterol free medium, their HMG - CoA reductase is strongly activated. In this experiment cells, cultivated in medium essentially sterol free, are treated with fluvastatin. A clear decrease in ROR $\alpha$  activity is observed, leading to the conclusion that the lowering of the intracellular cholesterol level is translated by a decrease of ROR $\alpha$  transcriptional activity (Table 5). U2OS cells are transfected with expression vector for ROR $\alpha$  (ROR) together with a luciferase reporter gene bearing a consensus response element for ROR $\alpha$  (ROR $\alpha$ -tk-luc). Luciferase activity is assayed in cells from 6 well plates and related to the activity in cells transfected with or without treatment with fluvastatin. The results are normalized to the protein content.

Table 5:

Fluvastatin	Fold induction	$\pm$ SEM
Control	76	14
+ 5 $\mu$ M	48	7
Control	93	6
+ 10 $\mu$ M	38	2

#### Cholesterol sulfate inhibition of ROR $\alpha$ binding to RORE

Various cholesterol derivatives including cholesterol sulfate (cpd No. 12 in Table 6): are screened in essentially cholesterol-free medium for binding of ROR $\alpha$  to the RORE. The ROR $\alpha$  protein is expressed in the baculovirus system. The other compounds are: No. 2: 5 $\alpha$ -Cholestan-3-one (Steraloids C4550), 3: 4-Cholesten-3 $\alpha$ -ol (C6090), 4: 5-Cholesten-3 $\beta$ , 6-diol (C6418), 5: 5-Cholesten-3 $\beta$ , 7 $\alpha$ -diol 7-benzoate (C6425), 6: 5-Cholesten-3 $\beta$ , 7 $\beta$ -diol 7-benzoate (C6438), 7: 5-Cholesten-3 $\beta$ , 19-diol (C6470), 8: 5-, 25R-Cholesten-3 $\beta$ , 26-diol (C6570), 9: 5-Cholesten-24 $\beta$ -ethyl-3 $\beta$ -ol acetate (C6681), 10: 5-Cholesten-3 $\alpha$ -ol (C6730), 11: 5-Cholesten-3 $\beta$ -ol (C6760), 12: 5-Cholesten-3 $\beta$ -ol sulfate, sodium salt (C6905), 13: 7, (5 $\alpha$ )-Cholesten-3 $\beta$ -ol (C7400), 14: 7-Dehydrocholesterol (Fluka 30800). This indicates that cholesterol sulfate, as predicted by the X-ray structure, is able to displace cholesterol.

#### Effect of cholesterol and cholesterol derivative on ROR alpha transcriptional activity

We next establish whether in eukaryotic cells partially depleted of cholesterol, ROR $\alpha$  transcriptional activity can be reconstituted by addition of cholesterol. We therefore treat the cells with

hydroxypropyl- $\beta$ -cyclodextrin (HPCD), a cyclodextrin derivative known to function as a cholesterol shuttle. HPCD treatment is used in experiments aiming at the partial depletion of intracellular cholesterol. In order to prevent an increase of intracellular cholesterol through the activation of the mevalonate pathway, cells are also treated with lovastatin while they are fed with a medium containing LDL-free serum. Using a combination of HPCD and lovastatin we find that transcription of the RORE reporter is stimulated in response to cholesterol, epicholesterol and cholestanol and to an even greater extent by cholesterol sulfate and 7-dehydrocholesterol. In contrast all the hydroxycholesterols tested do not display significant activity and the cholesterol derivative 5-cholesten-24 $\beta$ -ethyl-3 $\beta$ -ol-acetate does not trigger any increase in ROR $\alpha$  transcriptional activity as compared to vehicle (Table 6). These data correlate well with docking studies on cholesterol derivatives using our X-ray structure of ROR $\alpha$ .

Table 6:

Compounds ( 10 $\mu$ M)	Fold induction	$\pm$ SEM
Control	1	0.1
Cholesterol	3.3	0.1
Epicholesterol	2.8	0.44
Cholestanol	2.4	0.14
7-Dehydrochol	4.6	0.33
22(R)-OH-Chol	1.2	0.11
25-OH-Chol	1.6	0.06
20(S)-OH-Chol	1.2	0.11
Chol. Sulfate	5.4	0.31
27-OH-Chol	1.5	0.14
5-Cholesten-24beta	1	0.05

#### Ligand exchange screening by mass spectrometry

(His)<sub>6</sub>ROR $\alpha$ -LBD269-556 is produced in Sf9 cells and purified by Ni-NTA chromatography followed by size exclusion chromatography. The protein in Tris-HCl buffer at a concentration of 135  $\mu$ M is incubated overnight at 4 °C, with a 10-fold molar excess of 25-hydroxycholesterol (5-cholesten-3beta, 25-diol) or cholesterol sulfate (5-cholesten-3beta-ol-sulfate). Prior to mass spectrometry analysis, the protein is subjected to fast buffer exchange in 50 mM ammonium acetate pH 7.0 by size exclusion chromatography using disposable CentriSpin 20 columns (Princeton Separations, Adelphia, NJ) according to manufacturer's instructions. Mass spectrometry is carried out using a Q-Tof (Micromass, Manchester, UK) quadrupole time-of-flight hybrid tandem mass spectrometer equipped with a Micromass Z-type electrospray ionization source (ESI). The acquisition mass range is typically m/z 1500-4500 in 5 seconds. The mass spectrometer is tuned in order to allow detection of multiply-

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charged species of non-covalent complexes. The source block temperature and desolvation temperature are kept at 50 °C and 80 °C, respectively. Sample cone voltage ( $V_c$ ) is set to 23 volts for standard measurements. In-source induced fragmentation experiments are performed by increasing  $V_c$  up to 100 volts. The protein solution is infused at a flow rate of 10  $\mu$ L/min. Data are recorded and processed using Masslynx software. Spectra are deconvoluted using MaxEnt analysis software (Micromass, Manchester, UK). The results show that both 25-OH cholesterol and cholesterol sulfate are able to fully displace cholesterol bound to the ROR-LBD. Moreover, the comparison at various cone-voltages ( $V_c$ ) between the ligand/ROR-LBD-complex and the apo-ROR-LBD (without ligand) indicates that cholesterol and 25-OH cholesterol have a similar stability versus in-source collisions. In contrast, the cholesterol sulfate/ROR-LBD complex is more stable than cholesterol or 25-OH cholesterol complex.

Crystallization and X-ray structure of the complex ROR(alpha)/cholesterol-sulfate at 2.20Å Resolution: An example of structure based design

All amino acid residues relating to the complex ROR(alpha)/cholesterol-sulfate (e.g. the attached coordinates of the complex with cholesterol-sulfate, Table 9) are numbered according to splice variant Alpha-1 (i.e. P35398-2) of SWISS-PROT entry P35398 (corresponding to the number of a given amino acid according to SWISS-PROT P35398-1 as set out in Figure 1 minus 33). All amino acid residues relating to the complex ROR(alpha)/cholesterol (e.g. the attached coordinates of the complex with cholesterol, Table 8) are numbered according to splice variant Alpha-2 (i.e. P35398-1) of SWISS-PROT entry P35398, except for Figures 7-11, where the numbering used is according to P35398-2, and except in the following discussion of the comparison with the cholesterol-sulfate complex. All amino acid residues specified in the claims are numbered according to splice variant Alpha-2 (i.e. P35398-1) of SWISS-PROT entry P35398, as set out in Figure 1.

The proposal that cholesterol-sulfate is a ligand of ROR(alpha) is a result of structure based design, using the previously determined X-ray structure of ROR(alpha)/cholesterol at 1.63Å resolution. In particular, the latter X-ray structure reveals that in the hydrophilic part of the LBP there is space for a substituent attached to the hydroxy-group of cholesterol, if water molecules are displaced. The presence of three arginines (Arg292, Arg370 and Arg367) and of two free backbone amide nitrogens (NH-Gln289 and NH-Tyr290) strongly suggests a negatively charged substituent with at least two hydrogen-bond acceptor functionalities (e.g. a sulfate-group). Docking studies lead to the prediction that cholesterol-sulfate should have higher affinity than cholesterol. Subsequently it is shown by MS-

analysis that indeed cholesterol bound to ROR(alpha) LBD could be exchanged with cholesterol-sulfate.

The complex ROR(alpha)/cholesterol-sulfate could now be cocrystallized and the X-ray structure of the complex is solved at 2.20Å resolution with an  $R_{\text{cryst}}$  of 19.4% and  $R_{\text{free}}$  of 21.9% for data from 20Å to 2.20Å. The observed binding mode shows the following features:

- 1.) Cholesterol-sulfate and cholesterol have similar overall modes of binding, but cholesterol-sulfate is displaced slightly (e.g. corresponding C3-atoms by 0.85Å) towards the hydrophilic, positively charged, part of the LBP. This can be explained by the optimization of electrostatic and hydrogen-bond interactions made by the sulfate-group.
- 2.) Seven well-ordered water molecules present for cholesterol in the hydrophilic part of the LBP have been displaced in the complex with cholesterol-sulfate. Only one conserved water molecule is still present which mediates interactions between the sulfate group and NH1-Arg367 and O-Ala330.
- 3.) The sulfate group makes direct hydrogen bond interactions with NH-Gln289, NH-Tyr290 and NH1-Arg370. This confirms the docking hypothesis, which led to the proposal of cholesterol-sulfate.
- 4.) The only significant changes in the protein parts of the complexes of ROR(alpha) with cholesterol and cholesterol-sulfate occur for the sidechain of Ile327 and the loop 1-2 (residues Gln289 and Tyr290).

#### *Molecular Biology, Fermentation, Purification and MS-analysis*

Generation of the construct (His)<sub>6</sub>RORα-LBD<sub>270-523</sub>, fermentation and purification are done as described above. The exchange of cholesterol by cholesterol-sulfate is done at 37°C and confirmed by MS-analysis: Cholesterol sulfate is dissolved at 50 mM in DMSO and added at 1.0 mM final concentration to the (His)<sub>6</sub>RORα LBD<sub>270-523</sub> solution at 73 μM. The resulting solution is incubated overnight at 37° C and further purified by size exclusion chromatography on a SPX75 column, before concentrating to 17.6 mg/ml for crystallization trials. MS determination of the native complex is done as described previously (Kallen *et al.*, Structure, Vol.10, 1697-1707, 2002). A control experiment is done by incubating the same amount of RORα LBD protein with 5% DMSO under identical conditions. The protein concentration is approximately 15 μM in 50mM AcONH<sub>4</sub>, pH 7.0. Both spectra are recorded under identical conditions with V<sub>c</sub> = 20 volts.

#### *Crystallization*

The protein used for crystallization is at 17.6 mg/ml, in 100mM NaCl, 50mM Tris-HCl pH7.5, 5mM DTT. An ab initio search for crystallization conditions is undertaken. Trials are performed using a

standard vapor diffusion hanging drop set-up, with VDX crystallization plates and siliconized microscope cover slips from Hampton Research. Crystallization droplets are set up at 4°C by mixing on the coverslips 1.0µl of the protein stock solution with 1.0µl of a crystallization solution.

*X-ray Data collection:* A single crystal of approximate dimensions 60µm x 60µm x 200µm is mounted with a nylon CryoLoop (Hampton Research) and flash-frozen in a cold nitrogen stream for X-ray data collection at 100K. Diffraction data are collected at the Swiss Light Source (operating at 300mA), beamline X06SA, using a Marresearch CCD detector and an incident monochromatic X-ray beam with 0.9200Å wavelength. In total, 226 images are collected with 1.0° rotation each, using an exposure time of 9sec per frame and a crystal-to-detector distance of 150mm. Raw diffraction data are processed and scaled with the HKL program suite version 1.96.1 (Otwinowski and Minor, 1996). The estimated B-factor by Wilson plot analysis is 32.9 Å<sup>2</sup>. Crystal data and data collection statistics are shown in Table 7:

Number of crystals	1
Space group	P2 <sub>1</sub>
Unit cell dimensions	a=54.4Å b=49.9Å c=60.7Å
No. of monomers / a.u.	1
Packing coefficient	3.0Å <sup>3</sup> /Da
Estimated solvent content	58%
Wavelength	0.9200Å
Temperature	100K
Resolution range	20.0 – 2.2Å
No. of observations	57,993
No. of unique reflections	16,541
<hr/> Overall <hr/>	
Resolution range	20.0-2.2Å
Data redundancy	3.5
Completeness	99.7%
< I/ σ (I) >	16.2
R <sub>merge</sub> on intensities	0.079

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Reflections with $I \geq 3\sigma(I)$	66.4%
Highest resolution shell	
Resolution range	2.28-2.20Å
Data redundancy	2.8
Completeness	99.4%
$\langle I / \sigma(I) \rangle$	1.9
$R_{\text{merge}}$ on intensities	0.362
Reflections with $I \geq 3\sigma(I)$	25.9%

**Structure determination and refinement:** The structure is determined using as starting model the coordinates of the complex ROR(alpha)/cholesterol refined to 1.63Å resolution. The program REFMAC version 5.0 (CCP4, Acta Crystallogr. D50, 760-763, 1994) is used for refinement. Bulk solvent correction, an initial anisotropic B factor correction and restrained isotropic atomic B-factor refinement are applied. The refinement target is the maximum-likelihood target using amplitudes. No sigma cut-off is applied on the structure factor amplitudes. Cross-validation is used throughout refinement using a test set comprising 5.0% (829) of the unique reflections. Water molecules are identified with the program ARP/wARP and selected based on difference peak height (greater than  $3.0\sigma$ ) and distance criteria. Water molecules with temperature factors greater than  $70\text{\AA}^2$  are rejected. The program O version 7.0 (A.Jones et al., 1991) is used for model rebuilding. The refinement statistics for the final model are shown in Table 2. The final model of the complex ROR(alpha)/cholesterol-sulfate has good geometry (rms bond lengths = 0.014Å, rms bond angles = 1.41°) and no residues are in a disallowed region of the Ramachandran plot.

**Crystallization, data collection:** The crystals used for data collection are obtained with a well solution composed of 0.2M  $\text{MgCl}_2$ , 16% w/v PEG4000, 0.1M Tris HCl, pH 8.5. The crystals reached maximal dimensions of up to 0.2 mm within 6 weeks. The complex of RORα LBD with cholesterol-sulfate is thus crystallized in a crystal form with  $a=54.4\text{\AA}$ ,  $b=49.9\text{\AA}$ ,  $c=60.7\text{\AA}$ ,  $\beta=97.8^\circ$ ,  $P2_1$  and 1 complex/asymmetric unit, which is similar to the crystal form previously obtained in the complex with cholesterol.

**Conformation of cholesterol-sulfate bound to ROR(alpha) and its interactions:** In general, the electron density is of excellent quality, except for amino acids 461-464 (L9-10), which has only weak density. The protein part of the refined model consists of the last two His-amino acids from the His-tag,

followed by the PreScission<sup>TM</sup>-site (LEVLFQG) and by amino acids 271-511 of the ROR $\alpha$ -LBD. The refined model also contains 256 water molecules and 1 cholesterol-sulfate molecule.

The sulfate group makes direct hydrogen bond interactions with NH-Gln289 (3.0Å), NH-Tyr290 (2.9Å) and a bidentate interaction with NH1-Arg370 (3.0Å, 3.1Å). A water-mediated interaction is made with NH1-Arg367.

*Comparison of the X-ray structures of cholesterol-sulfate and cholesterol bound to ROR(alpha) LBD*

Figure 10 shows a superposition (using C $\alpha$ 's of the respective LBD's) for the ROR(alpha) complexes with cholesterol and cholesterol-sulfate. The r.m.s.d for the C $\alpha$  atoms of residues Pro270-Phe511 after superposition is 0.26Å. The only significant changes in the protein parts occur for the sidechain of Ile327 and the loop 1-2 (residues Gln289 and Tyr290): The backbone NH-atoms for Gln289 and Tyr290 move by ca. 0.8Å towards the sulfate-group (with a concomitant movement of the respective sidechains), in order to improve the interactions with the sulfate-group. The sidechain of Ile327 has to move slightly, in order to avoid a steric clash with the terminal isopropyl-group (Figure .9). The comparison shows that cholesterol-sulfate and cholesterol have similar overall modes of binding, but cholesterol-sulfate is displaced slightly (e.g. corresponding C3-atoms by 0.85Å and corresponding C2-atoms by 0.7Å) towards the hydrophilic, positively charged, part of the LBP (Figure 9). This can be explained by the optimization of electrostatic and hydrogen-bond interactions made by the sulfate-group. 7 well-ordered water molecules present for cholesterol in the hydrophilic part of the LBP have been displaced in the complex with cholesterol-sulfate (Figure 10). Only one conserved water molecule is still present which mediates interactions between the sulfate group and NH1-Arg367 and O-Ala330. The sulfate group makes direct hydrogen bond interactions with NH-Gln289, NH-Tyr290 and NH1-Arg370. This confirms the docking hypothesis, which led to the proposal of cholesterol-sulfate.

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TABLE 8

ATOM	1	CB	HIS	A	308	-3.470	26.612	-1.587	1.00	57.47
ATOM	2	CG	HIS	A	308	-4.960	26.750	-1.571	1.00	68.25
ATOM	3	CD2	HIS	A	308	-5.766	27.800	-1.862	1.00	72.02
ATOM	4	ND1	HIS	A	308	-5.794	25.720	-1.190	1.00	71.55
ATOM	5	CE1	HIS	A	308	-7.049	26.131	-1.245	1.00	75.57
ATOM	6	NE2	HIS	A	308	-7.061	27.389	-1.652	1.00	73.93
ATOM	7	C	HIS	A	308	-1.527	26.518	-0.048	1.00	46.68
ATOM	8	O	HIS	A	308	-1.408	25.970	1.039	1.00	46.34
ATOM	9	N	HIS	A	308	-2.472	28.682	-0.665	1.00	46.21
ATOM	10	CA	HIS	A	308	-2.791	27.256	-0.390	1.00	50.95
ATOM	11	N	LEU	A	309	-0.598	26.489	-0.995	1.00	43.13
ATOM	12	CA	LEU	A	309	0.692	25.856	-0.780	1.00	43.49
ATOM	13	CB	LEU	A	309	1.517	25.900	-2.069	1.00	41.03
ATOM	14	CG	LEU	A	309	2.967	25.402	-2.033	1.00	39.69
ATOM	15	CD1	LEU	A	309	2.988	23.898	-1.765	1.00	39.26
ATOM	16	CD2	LEU	A	309	3.668	25.742	-3.348	1.00	33.46
ATOM	17	C	LEU	A	309	1.397	26.673	0.307	1.00	41.27
ATOM	18	O	LEU	A	309	1.987	26.121	1.217	1.00	39.43
ATOM	19	N	ALA	A	310	1.371	27.994	0.158	1.00	41.63
ATOM	20	CA	ALA	A	310	1.972	28.894	1.125	1.00	43.60
ATOM	21	CB	ALA	A	310	1.772	30.334	0.692	1.00	41.23
ATOM	22	C	ALA	A	310	1.324	28.638	2.494	1.00	44.99
ATOM	23	O	ALA	A	310	2.028	28.454	3.487	1.00	42.70
ATOM	24	N	GLN	A	311	-0.011	28.589	2.531	1.00	46.22
ATOM	25	CA	GLN	A	311	-0.765	28.330	3.767	1.00	48.70
ATOM	26	CB	GLN	A	311	-2.266	28.239	3.472	1.00	55.01
ATOM	27	CG	GLN	A	311	-3.081	29.513	3.686	1.00	69.31
ATOM	28	CD	GLN	A	311	-4.596	29.289	3.479	1.00	78.89
ATOM	29	OE1	GLN	A	311	-5.137	28.224	3.832	1.00	83.81
ATOM	30	NE2	GLN	A	311	-5.275	30.278	2.876	1.00	82.00
ATOM	31	C	GLN	A	311	-0.339	27.015	4.413	1.00	45.78
ATOM	32	O	GLN	A	311	-0.043	26.949	5.599	1.00	43.47
ATOM	33	N	ASN	A	312	-0.332	25.966	3.604	1.00	43.80
ATOM	34	CA	ASN	A	312	0.023	24.624	4.049	1.00	43.06
ATOM	35	CB	ASN	A	312	-0.236	23.632	2.918	1.00	52.50
ATOM	36	CG	ASN	A	312	0.867	22.607	2.776	1.00	64.44
ATOM	37	OD1	ASN	A	312	0.709	21.453	3.173	1.00	73.51
ATOM	38	ND2	ASN	A	312	1.992	23.017	2.191	1.00	70.50
ATOM	39	C	ASN	A	312	1.437	24.436	4.606	1.00	40.68
ATOM	40	O	ASN	A	312	1.635	23.638	5.518	1.00	39.27
ATOM	41	N	ILE	A	313	2.424	25.072	3.974	1.00	39.40
ATOM	42	CA	ILE	A	313	3.824	24.979	4.407	1.00	38.82
ATOM	43	CB	ILE	A	313	4.802	25.421	3.253	1.00	34.58
ATOM	44	CG2	ILE	A	313	6.169	25.806	3.799	1.00	36.01
ATOM	45	CG1	ILE	A	313	4.956	24.284	2.240	1.00	37.16
ATOM	46	CD1	ILE	A	313	6.005	24.537	1.154	1.00	35.61
ATOM	47	C	ILE	A	313	4.030	25.798	5.703	1.00	37.29
ATOM	48	O	ILE	A	313	4.786	25.399	6.585	1.00	39.16
ATOM	49	N	SER	A	314	3.298	26.906	5.823	1.00	35.32
ATOM	50	CA	SER	A	314	3.334	27.790	6.989	1.00	36.43
ATOM	51	CB	SER	A	314	2.457	29.014	6.728	1.00	37.35
ATOM	52	OG	SER	A	314	3.059	29.848	5.759	1.00	41.24
ATOM	53	C	SER	A	314	2.807	27.089	8.241	1.00	35.85
ATOM	54	O	SER	A	314	3.305	27.283	9.351	1.00	36.16
ATOM	55	N	LYS	A	315	1.777	26.288	8.033	1.00	35.61
ATOM	56	CA	LYS	A	315	1.131	25.547	9.094	1.00	36.35
ATOM	57	CB	LYS	A	315	-0.183	24.969	8.564	1.00	34.96
ATOM	58	CG	LYS	A	315	-1.051	24.316	9.597	1.00	38.82
ATOM	59	CD	LYS	A	315	-2.470	24.232	9.084	1.00	49.73
ATOM	60	CE	LYS	A	315	-3.386	23.556	10.082	1.00	56.14
ATOM	61	NZ	LYS	A	315	-3.021	22.113	10.247	1.00	65.23
ATOM	62	C	LYS	A	315	2.056	24.438	9.571	1.00	36.74
ATOM	63	O	LYS	A	315	2.102	24.130	10.757	1.00	38.14



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ATOM	64	N	SER A 316	2.771	23.835	8.624	1.00	35.23
ATOM	65	CA	SER A 316	3.708	22.757	8.904	1.00	31.03
ATOM	66	CB	SER A 316	4.268	22.189	7.591	1.00	33.89
ATOM	67	OG	SER A 316	3.275	21.504	6.838	1.00	36.00
ATOM	68	C	SER A 316	4.842	23.293	9.769	1.00	31.80
ATOM	69	O	SER A 316	5.223	22.667	10.760	1.00	30.02
ATOM	70	N	HIS A 317	5.391	24.440	9.354	1.00	29.40
ATOM	71	CA	HIS A 317	6.468	25.128	10.078	1.00	31.38
ATOM	72	CB	HIS A 317	6.838	26.397	9.319	1.00	28.86
ATOM	73	CG	HIS A 317	7.765	27.317	10.058	1.00	30.88
ATOM	74	CD2	HIS A 317	7.590	28.583	10.506	1.00	31.39
ATOM	75	ND1	HIS A 317	9.085	27.007	10.310	1.00	31.14
ATOM	76	CE1	HIS A 317	9.686	28.042	10.866	1.00	29.44
ATOM	77	NE2	HIS A 317	8.801	29.012	10.996	1.00	30.99
ATOM	78	C	HIS A 317	5.964	25.489	11.486	1.00	32.96
ATOM	79	O	HIS A 317	6.647	25.271	12.491	1.00	30.21
ATOM	80	N	LEU A 318	4.766	26.066	11.519	1.00	35.80
ATOM	81	CA	LEU A 318	4.099	26.456	12.754	1.00	39.30
ATOM	82	CB	LEU A 318	2.651	26.888	12.454	1.00	42.10
ATOM	83	CG	LEU A 318	1.664	27.026	13.629	1.00	45.53
ATOM	84	CD1	LEU A 318	1.898	28.331	14.354	1.00	42.84
ATOM	85	CD2	LEU A 318	0.233	26.963	13.127	1.00	46.58
ATOM	86	C	LEU A 318	4.070	25.267	13.708	1.00	39.53
ATOM	87	O	LEU A 318	4.581	25.337	14.829	1.00	45.11
ATOM	88	N	GLU A 319	3.517	24.157	13.235	1.00	34.75
ATOM	89	CA	GLU A 319	3.378	22.951	14.040	1.00	31.78
ATOM	90	CB	GLU A 319	2.258	22.088	13.464	1.00	35.64
ATOM	91	CG	GLU A 319	0.966	22.887	13.304	1.00	43.85
ATOM	92	CD	GLU A 319	-0.204	22.079	12.797	1.00	48.29
ATOM	93	OE1	GLU A 319	-0.046	20.870	12.496	1.00	51.24
ATOM	94	OE2	GLU A 319	-1.299	22.675	12.715	1.00	49.93
ATOM	95	C	GLU A 319	4.605	22.092	14.335	1.00	31.28
ATOM	96	O	GLU A 319	4.501	21.150	15.128	1.00	29.74
ATOM	97	N	THR A 320	5.749	22.374	13.703	1.00	29.30
ATOM	98	CA	THR A 320	6.948	21.589	13.957	1.00	25.31
ATOM	99	CB	THR A 320	7.428	20.826	12.723	1.00	26.81
ATOM	100	OG1	THR A 320	7.760	21.760	11.697	1.00	31.74
ATOM	101	CG2	THR A 320	6.371	19.874	12.228	1.00	25.26
ATOM	102	C	THR A 320	8.086	22.435	14.499	1.00	27.08
ATOM	103	O	THR A 320	9.251	22.078	14.369	1.00	28.40
ATOM	104	N	CYS A 321	7.754	23.591	15.058	1.00	27.84
ATOM	105	CA	CYS A 321	8.758	24.440	15.690	1.00	32.58
ATOM	106	CB	CYS A 321	8.575	25.897	15.291	1.00	35.52
ATOM	107	SG	CYS A 321	9.587	26.379	13.907	1.00	31.41
ATOM	108	C	CYS A 321	8.481	24.273	17.183	1.00	33.42
ATOM	109	O	CYS A 321	7.315	24.272	17.584	1.00	33.09
ATOM	110	N	GLN A 322	9.516	24.122	18.005	1.00	33.42
ATOM	111	CA	GLN A 322	9.280	23.945	19.435	1.00	37.77
ATOM	112	CB	GLN A 322	10.566	23.575	20.159	1.00	38.95
ATOM	113	CG	GLN A 322	10.311	23.332	21.638	1.00	41.00
ATOM	114	CD	GLN A 322	11.474	22.709	22.355	1.00	43.45
ATOM	115	OE1	GLN A 322	12.639	22.892	21.974	1.00	45.86
ATOM	116	NE2	GLN A 322	11.173	21.973	23.408	1.00	43.47
ATOM	117	C	GLN A 322	8.595	25.133	20.143	1.00	38.21
ATOM	118	O	GLN A 322	7.627	24.945	20.891	1.00	40.89
ATOM	119	N	TYR A 323	9.087	26.348	19.893	1.00	37.01
ATOM	120	CA	TYR A 323	8.518	27.545	20.513	1.00	39.53
ATOM	121	CB	TYR A 323	9.576	28.318	21.306	1.00	37.75
ATOM	122	CG	TYR A 323	10.245	27.509	22.370	1.00	36.25
ATOM	123	CD1	TYR A 323	11.551	27.058	22.191	1.00	40.18
ATOM	124	CE1	TYR A 323	12.185	26.279	23.139	1.00	43.63
ATOM	125	CD2	TYR A 323	9.576	27.164	23.537	1.00	38.29
ATOM	126	CE2	TYR A 323	10.196	26.386	24.500	1.00	43.87
ATOM	127	CZ	TYR A 323	11.508	25.945	24.294	1.00	45.72
ATOM	128	OH	TYR A 323	12.165	25.182	25.236	1.00	50.91
ATOM	129	C	TYR A 323	7.916	28.496	19.502	1.00	41.39

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ATOM	130	O	TYR	A	323	8.185	28.404	18.302	1.00	43.21
ATOM	131	N	LEU	A	324	7.149	29.451	20.011	1.00	38.45
ATOM	132	CA	LEU	A	324	6.556	30.442	19.158	1.00	36.36
ATOM	133	CB	LEU	A	324	5.260	30.960	19.761	1.00	40.65
ATOM	134	CG	LEU	A	324	4.135	29.917	19.804	1.00	47.37
ATOM	135	CD1	LEU	A	324	3.021	30.333	20.790	1.00	48.02
ATOM	136	CD2	LEU	A	324	3.569	29.698	18.390	1.00	48.49
ATOM	137	C	LEU	A	324	7.586	31.548	19.037	1.00	36.82
ATOM	138	O	LEU	A	324	8.369	31.791	19.955	1.00	35.71
ATOM	139	N	ARG	A	325	7.604	32.185	17.876	1.00	33.86
ATOM	140	CA	ARG	A	325	8.519	33.274	17.595	1.00	34.00
ATOM	141	CB	ARG	A	325	8.132	33.913	16.252	1.00	32.60
ATOM	142	CG	ARG	A	325	9.087	34.947	15.744	1.00	29.17
ATOM	143	CD	ARG	A	325	10.477	34.371	15.667	1.00	30.77
ATOM	144	NE	ARG	A	325	11.388	35.268	14.984	1.00	31.48
ATOM	145	CZ	ARG	A	325	11.340	35.518	13.681	1.00	41.33
ATOM	146	NH1	ARG	A	325	10.421	34.931	12.912	1.00	39.89
ATOM	147	NH2	ARG	A	325	12.195	36.383	13.147	1.00	42.61
ATOM	148	C	ARG	A	325	8.462	34.328	18.711	1.00	36.35
ATOM	149	O	ARG	A	325	9.503	34.826	19.145	1.00	37.18
ATOM	150	N	GLU	A	326	7.244	34.639	19.169	1.00	39.65
ATOM	151	CA	GLU	A	326	6.985	35.626	20.226	1.00	41.32
ATOM	152	CB	GLU	A	326	5.487	35.784	20.459	1.00	46.07
ATOM	153	CG	GLU	A	326	4.720	36.379	19.272	1.00	65.71
ATOM	154	CD	GLU	A	326	4.555	35.424	18.062	1.00	72.41
ATOM	155	OE1	GLU	A	326	4.261	34.214	18.267	1.00	74.04
ATOM	156	OE2	GLU	A	326	4.696	35.904	16.901	1.00	73.55
ATOM	157	C	GLU	A	326	7.659	35.211	21.520	1.00	38.16
ATOM	158	O	GLU	A	326	8.332	36.023	22.148	1.00	35.77
ATOM	159	N	GLU	A	327	7.487	33.938	21.880	1.00	35.48
ATOM	160	CA	GLU	A	327	8.092	33.353	23.077	1.00	38.23
ATOM	161	CB	GLU	A	327	7.911	31.833	23.082	1.00	46.45
ATOM	162	CG	GLU	A	327	6.486	31.293	23.134	1.00	57.52
ATOM	163	CD	GLU	A	327	6.452	29.752	23.125	1.00	63.49
ATOM	164	OE1	GLU	A	327	7.441	29.113	23.557	1.00	68.14
ATOM	165	OE2	GLU	A	327	5.445	29.172	22.667	1.00	68.00
ATOM	166	C	GLU	A	327	9.599	33.615	23.140	1.00	34.14
ATOM	167	O	GLU	A	327	10.098	34.218	24.076	1.00	34.19
ATOM	168	N	LEU	A	328	10.304	33.158	22.114	1.00	29.72
ATOM	169	CA	LEU	A	328	11.748	33.293	22.006	1.00	29.32
ATOM	170	CB	LEU	A	328	12.217	32.636	20.712	1.00	29.59
ATOM	171	CG	LEU	A	328	12.016	31.131	20.626	1.00	30.01
ATOM	172	CD1	LEU	A	328	11.986	30.725	19.164	1.00	31.46
ATOM	173	CD2	LEU	A	328	13.119	30.432	21.367	1.00	22.42
ATOM	174	C	LEU	A	328	12.267	34.715	22.041	1.00	28.85
ATOM	175	O	LEU	A	328	13.366	34.954	22.518	1.00	29.43
ATOM	176	N	GLN	A	329	11.486	35.654	21.520	1.00	33.80
ATOM	177	CA	GLN	A	329	11.901	37.056	21.481	1.00	37.54
ATOM	178	CB	GLN	A	329	11.093	37.808	20.439	1.00	43.64
ATOM	179	CG	GLN	A	329	11.132	37.198	19.050	1.00	53.22
ATOM	180	CD	GLN	A	329	10.283	37.983	18.065	1.00	59.04
ATOM	181	OE1	GLN	A	329	9.035	37.966	18.127	1.00	59.51
ATOM	182	NE2	GLN	A	329	10.953	38.720	17.174	1.00	59.14
ATOM	183	C	GLN	A	329	11.725	37.721	22.846	1.00	35.96
ATOM	184	O	GLN	A	329	12.525	38.562	23.241	1.00	30.61
ATOM	185	N	GLN	A	330	10.695	37.308	23.572	1.00	36.62
ATOM	186	CA	GLN	A	330	10.450	37.846	24.901	1.00	41.09
ATOM	187	CB	GLN	A	330	9.093	37.383	25.391	1.00	45.78
ATOM	188	CG	GLN	A	330	7.957	37.930	24.579	1.00	63.61
ATOM	189	CD	GLN	A	330	6.686	37.133	24.784	1.00	74.77
ATOM	190	OE1	GLN	A	330	6.569	36.365	25.750	1.00	79.50
ATOM	191	NE2	GLN	A	330	5.730	37.285	23.865	1.00	82.47
ATOM	192	C	GLN	A	330	11.515	37.477	25.951	1.00	38.55
ATOM	193	O	GLN	A	330	11.609	38.135	26.979	1.00	41.30
ATOM	194	N	ILE	A	331	12.305	36.429	25.715	1.00	32.00
ATOM	195	CA	ILE	A	331	13.313	36.015	26.686	1.00	23.76

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ATOM	196	CB	ILE	A	331	13.078	34.596	27.169	1.00	22.66
ATOM	197	CG2	ILE	A	331	11.656	34.435	27.630	1.00	21.34
ATOM	198	CG1	ILE	A	331	13.355	33.619	26.053	1.00	24.33
ATOM	199	CD1	ILE	A	331	13.364	32.235	26.555	1.00	23.84
ATOM	200	C	ILE	A	331	14.738	36.183	26.205	1.00	23.46
ATOM	201	O	ILE	A	331	15.657	35.455	26.592	1.00	27.34
ATOM	202	N	THR	A	332	14.918	37.180	25.354	1.00	23.06
ATOM	203	CA	THR	A	332	16.204	37.521	24.799	1.00	23.34
ATOM	204	CB	THR	A	332	15.962	38.552	23.680	1.00	31.64
ATOM	205	OG1	THR	A	332	16.261	37.954	22.404	1.00	35.81
ATOM	206	CG2	THR	A	332	16.735	39.863	23.912	1.00	37.99
ATOM	207	C	THR	A	332	17.180	38.051	25.857	1.00	20.21
ATOM	208	O	THR	A	332	18.401	37.887	25.749	1.00	21.02
ATOM	209	N	TRP	A	333	16.628	38.683	26.886	1.00	25.18
ATOM	210	CA	TRP	A	333	17.437	39.226	27.988	1.00	23.07
ATOM	211	CB	TRP	A	333	16.582	40.108	28.879	1.00	19.83
ATOM	212	CG	TRP	A	333	15.407	39.426	29.504	1.00	17.19
ATOM	213	CD2	TRP	A	333	15.344	38.851	30.820	1.00	22.36
ATOM	214	CE2	TRP	A	333	14.030	38.392	31.008	1.00	26.11
ATOM	215	CE3	TRP	A	333	16.274	38.693	31.865	1.00	22.59
ATOM	216	CD1	TRP	A	333	14.172	39.294	28.974	1.00	14.35
ATOM	217	NE1	TRP	A	333	13.336	38.671	29.858	1.00	19.63
ATOM	218	CZ2	TRP	A	333	13.607	37.778	32.213	1.00	25.43
ATOM	219	CZ3	TRP	A	333	15.852	38.082	33.056	1.00	21.23
ATOM	220	CH2	TRP	A	333	14.538	37.636	33.216	1.00	20.18
ATOM	221	C	TRP	A	333	18.028	38.116	28.826	1.00	23.38
ATOM	222	O	TRP	A	333	19.030	38.314	29.500	1.00	27.96
ATOM	223	N	GLN	A	334	17.436	36.925	28.730	1.00	24.06
ATOM	224	CA	GLN	A	334	17.893	35.767	29.492	1.00	22.85
ATOM	225	CB	GLN	A	334	16.804	34.712	29.586	1.00	22.07
ATOM	226	CG	GLN	A	334	15.575	35.251	30.240	1.00	25.58
ATOM	227	CD	GLN	A	334	14.492	34.228	30.427	1.00	29.55
ATOM	228	OE1	GLN	A	334	14.621	33.066	30.029	1.00	32.54
ATOM	229	NE2	GLN	A	334	13.388	34.664	31.006	1.00	31.52
ATOM	230	C	GLN	A	334	19.169	35.145	29.016	1.00	23.02
ATOM	231	O	GLN	A	334	19.180	34.020	28.519	1.00	27.49
ATOM	232	N	THR	A	335	20.257	35.878	29.179	1.00	21.73
ATOM	233	CA	THR	A	335	21.566	35.403	28.804	1.00	20.96
ATOM	234	CB	THR	A	335	22.436	36.595	28.396	1.00	26.82
ATOM	235	OG1	THR	A	335	22.471	37.528	29.487	1.00	25.70
ATOM	236	CG2	THR	A	335	21.881	37.286	27.109	1.00	18.02
ATOM	237	C	THR	A	335	22.237	34.647	29.978	1.00	24.27
ATOM	238	O	THR	A	335	21.794	34.762	31.133	1.00	25.14
ATOM	239	N	PHE	A	336	23.306	33.902	29.682	1.00	22.91
ATOM	240	CA	PHE	A	336	24.048	33.138	30.693	1.00	27.78
ATOM	241	CB	PHE	A	336	25.036	32.126	30.051	1.00	23.18
ATOM	242	CG	PHE	A	336	24.385	30.861	29.569	1.00	24.30
ATOM	243	CD1	PHE	A	336	24.236	30.615	28.193	1.00	24.39
ATOM	244	CD2	PHE	A	336	23.855	29.952	30.477	1.00	18.74
ATOM	245	CE1	PHE	A	336	23.558	29.484	27.734	1.00	19.18
ATOM	246	CE2	PHE	A	336	23.174	28.824	30.043	1.00	20.30
ATOM	247	CZ	PHE	A	336	23.018	28.582	28.667	1.00	24.72
ATOM	248	C	PHE	A	336	24.835	34.058	31.632	1.00	30.11
ATOM	249	O	PHE	A	336	25.560	34.953	31.182	1.00	27.94
ATOM	250	N	LEU	A	337	24.682	33.840	32.934	1.00	29.31
ATOM	251	CA	LEU	A	337	25.413	34.631	33.921	1.00	30.51
ATOM	252	CB	LEU	A	337	24.920	34.293	35.339	1.00	30.83
ATOM	253	CG	LEU	A	337	23.426	34.451	35.652	1.00	27.00
ATOM	254	CD1	LEU	A	337	23.096	33.895	37.023	1.00	28.96
ATOM	255	CD2	LEU	A	337	23.047	35.915	35.568	1.00	29.51
ATOM	256	C	LEU	A	337	26.902	34.311	33.755	1.00	30.04
ATOM	257	O	LEU	A	337	27.247	33.289	33.180	1.00	31.12
ATOM	258	N	GLN	A	338	27.779	35.200	34.226	1.00	32.35
ATOM	259	CA	GLN	A	338	29.231	35.036	34.098	1.00	32.95
ATOM	260	CB	GLN	A	338	29.954	36.189	34.782	1.00	36.81
ATOM	261	CG	GLN	A	338	31.330	36.423	34.214	1.00	45.74

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ATOM	262	CD	GLN	A	338	31.292	36.625	32.691	1.00	60.39
ATOM	263	OE1	GLN	A	338	30.414	37.330	32.158	1.00	62.23
ATOM	264	NE2	GLN	A	338	32.237	35.995	31.985	1.00	63.44
ATOM	265	C	GLN	A	338	29.810	33.731	34.616	1.00	32.21
ATOM	266	O	GLN	A	338	30.818	33.230	34.122	1.00	31.25
ATOM	267	N	GLU	A	339	29.212	33.234	35.681	1.00	33.70
ATOM	268	CA	GLU	A	339	29.655	31.989	36.297	1.00	35.07
ATOM	269	CB	GLU	A	339	28.889	31.747	37.611	1.00	42.66
ATOM	270	CG	GLU	A	339	28.630	33.037	38.449	1.00	55.90
ATOM	271	CD	GLU	A	339	27.288	33.741	38.127	1.00	58.95
ATOM	272	OE1	GLU	A	339	27.183	34.992	38.255	1.00	47.67
ATOM	273	OE2	GLU	A	339	26.325	33.023	37.771	1.00	67.60
ATOM	274	C	GLU	A	339	29.340	30.878	35.319	1.00	27.81
ATOM	275	O	GLU	A	339	30.156	30.016	35.062	1.00	26.00
ATOM	276	N	GLU	A	340	28.125	30.906	34.795	1.00	26.98
ATOM	277	CA	GLU	A	340	27.678	29.911	33.831	1.00	28.10
ATOM	278	CB	GLU	A	340	26.223	30.163	33.457	1.00	29.51
ATOM	279	CG	GLU	A	340	25.282	30.053	34.636	1.00	26.99
ATOM	280	CD	GLU	A	340	23.849	30.355	34.284	1.00	30.46
ATOM	281	OE1	GLU	A	340	22.970	29.488	34.510	1.00	34.56
ATOM	282	OE2	GLU	A	340	23.580	31.471	33.802	1.00	31.24
ATOM	283	C	GLU	A	340	28.573	29.875	32.592	1.00	25.22
ATOM	284	O	GLU	A	340	28.910	28.798	32.096	1.00	24.52
ATOM	285	N	ILE	A	341	29.008	31.039	32.126	1.00	23.36
ATOM	286	CA	ILE	A	341	29.878	31.070	30.953	1.00	28.31
ATOM	287	CB	ILE	A	341	30.087	32.544	30.391	1.00	27.91
ATOM	288	CG2	ILE	A	341	31.242	32.598	29.382	1.00	23.19
ATOM	289	CG1	ILE	A	341	28.799	33.040	29.718	1.00	26.01
ATOM	290	CD1	ILE	A	341	28.772	34.533	29.426	1.00	26.73
ATOM	291	C	ILE	A	341	31.210	30.382	31.208	1.00	29.36
ATOM	292	O	ILE	A	341	31.682	29.598	30.388	1.00	29.02
ATOM	293	N	GLU	A	342	31.800	30.642	32.372	1.00	36.68
ATOM	294	CA	GLU	A	342	33.101	30.052	32.700	1.00	37.76
ATOM	295	CB	GLU	A	342	33.692	30.615	34.011	1.00	50.01
ATOM	296	CG	GLU	A	342	32.840	30.441	35.298	1.00	68.37
ATOM	297	CD	GLU	A	342	32.978	29.073	36.006	1.00	77.44
ATOM	298	OE1	GLU	A	342	34.115	28.691	36.384	1.00	81.72
ATOM	299	OE2	GLU	A	342	31.938	28.398	36.218	1.00	79.74
ATOM	300	C	GLU	A	342	32.969	28.567	32.793	1.00	29.07
ATOM	301	O	GLU	A	342	33.873	27.835	32.421	1.00	25.34
ATOM	302	N	ASN	A	343	31.832	28.138	33.316	1.00	28.65
ATOM	303	CA	ASN	A	343	31.581	26.729	33.459	1.00	31.12
ATOM	304	CB	ASN	A	343	30.239	26.495	34.113	1.00	31.12
ATOM	305	CG	ASN	A	343	29.952	25.051	34.268	1.00	44.07
ATOM	306	OD1	ASN	A	343	30.740	24.315	34.857	1.00	52.87
ATOM	307	ND2	ASN	A	343	28.870	24.593	33.658	1.00	49.75
ATOM	308	C	ASN	A	343	31.693	26.050	32.091	1.00	31.48
ATOM	309	O	ASN	A	343	32.474	25.106	31.939	1.00	32.73
ATOM	310	N	TYR	A	344	30.980	26.578	31.089	1.00	31.34
ATOM	311	CA	TYR	A	344	31.056	26.028	29.720	1.00	27.38
ATOM	312	CB	TYR	A	344	30.133	26.778	28.747	1.00	19.95
ATOM	313	CG	TYR	A	344	28.678	26.486	28.906	1.00	15.00
ATOM	314	CD1	TYR	A	344	27.802	27.473	29.313	1.00	12.78
ATOM	315	CE1	TYR	A	344	26.453	27.216	29.464	1.00	15.93
ATOM	316	CD2	TYR	A	344	28.169	25.217	28.649	1.00	16.37
ATOM	317	CE2	TYR	A	344	26.805	24.939	28.802	1.00	17.65
ATOM	318	CZ	TYR	A	344	25.953	25.946	29.210	1.00	14.48
ATOM	319	OH	TYR	A	344	24.612	25.705	29.377	1.00	15.05
ATOM	320	C	TYR	A	344	32.467	26.132	29.189	1.00	27.55
ATOM	321	O	TYR	A	344	32.966	25.216	28.542	1.00	30.70
ATOM	322	N	GLN	A	345	33.125	27.253	29.451	1.00	28.25
ATOM	323	CA	GLN	A	345	34.474	27.392	28.940	1.00	31.21
ATOM	324	CB	GLN	A	345	34.982	28.819	29.063	1.00	29.90
ATOM	325	CG	GLN	A	345	34.201	29.825	28.254	1.00	35.96
ATOM	326	CD	GLN	A	345	34.801	31.209	28.343	1.00	40.32
ATOM	327	OE1	GLN	A	345	35.654	31.469	29.187	1.00	43.48

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ATOM	328	NE2	GLN	A	345	34.375	32.101	27.469	1.00	40.57
ATOM	329	C	GLN	A	345	35.397	26.446	29.668	1.00	36.16
ATOM	330	O	GLN	A	345	36.485	26.128	29.179	1.00	36.49
ATOM	331	N	ASN	A	346	34.972	26.004	30.853	1.00	42.02
ATOM	332	CA	ASN	A	346	35.780	25.077	31.630	1.00	42.72
ATOM	333	CB	ASN	A	346	35.532	25.237	33.135	1.00	48.26
ATOM	334	CG	ASN	A	346	36.336	26.398	33.743	1.00	52.40
ATOM	335	OD1	ASN	A	346	37.433	26.728	33.282	1.00	53.04
ATOM	336	ND2	ASN	A	346	35.802	26.995	34.799	1.00	53.36
ATOM	337	C	ASN	A	346	35.633	23.619	31.189	1.00	40.45
ATOM	338	O	ASN	A	346	36.533	22.810	31.475	1.00	38.19
ATOM	339	N	LYS	A	347	34.559	23.293	30.449	1.00	32.64
ATOM	340	CA	LYS	A	347	34.351	21.912	29.980	1.00	26.11
ATOM	341	CB	LYS	A	347	32.985	21.742	29.338	1.00	22.43
ATOM	342	CG	LYS	A	347	31.860	22.141	30.218	1.00	21.17
ATOM	343	CD	LYS	A	347	30.533	21.903	29.569	1.00	25.53
ATOM	344	CE	LYS	A	347	29.436	22.235	30.550	1.00	31.64
ATOM	345	NZ	LYS	A	347	28.105	21.911	30.002	1.00	42.98
ATOM	346	C	LYS	A	347	35.417	21.514	28.979	1.00	25.51
ATOM	347	O	LYS	A	347	35.862	22.338	28.186	1.00	30.14
ATOM	348	N	GLN	A	348	35.873	20.269	29.058	1.00	23.11
ATOM	349	CA	GLN	A	348	36.891	19.771	28.128	1.00	29.12
ATOM	350	CB	GLN	A	348	37.252	18.338	28.502	1.00	37.39
ATOM	351	CG	GLN	A	348	37.330	18.100	30.007	1.00	50.83
ATOM	352	CD	GLN	A	348	38.742	17.956	30.494	1.00	55.85
ATOM	353	OE1	GLN	A	348	39.428	17.011	30.122	1.00	61.65
ATOM	354	NE2	GLN	A	348	39.190	18.883	31.342	1.00	65.17
ATOM	355	C	GLN	A	348	36.292	19.803	26.704	1.00	25.62
ATOM	356	O	GLN	A	348	35.067	19.729	26.570	1.00	25.40
ATOM	357	N	ARG	A	349	37.137	19.854	25.668	1.00	28.86
ATOM	358	CA	ARG	A	349	36.671	19.928	24.271	1.00	30.13
ATOM	359	CB	ARG	A	349	37.831	19.768	23.276	1.00	38.59
ATOM	360	CG	ARG	A	349	37.408	20.068	21.821	1.00	51.14
ATOM	361	CD	ARG	A	349	38.539	19.932	20.772	1.00	60.22
ATOM	362	NE	ARG	A	349	38.121	20.510	19.481	1.00	71.23
ATOM	363	CZ	ARG	A	349	38.525	20.126	18.263	1.00	72.91
ATOM	364	NH1	ARG	A	349	39.392	19.130	18.090	1.00	72.73
ATOM	365	NH2	ARG	A	349	38.041	20.753	17.198	1.00	71.22
ATOM	366	C	ARG	A	349	35.578	18.940	23.908	1.00	28.40
ATOM	367	O	ARG	A	349	34.527	19.322	23.387	1.00	26.63
ATOM	368	N	GLU	A	350	35.857	17.662	24.165	1.00	29.38
ATOM	369	CA	GLU	A	350	34.932	16.565	23.877	1.00	27.83
ATOM	370	CB	GLU	A	350	35.586	15.215	24.184	1.00	33.12
ATOM	371	CG	GLU	A	350	35.794	14.956	25.684	1.00	35.99
ATOM	372	CD	GLU	A	350	37.212	15.247	26.148	1.00	38.01
ATOM	373	OE1	GLU	A	350	37.736	14.408	26.913	1.00	43.71
ATOM	374	OE2	GLU	A	350	37.809	16.283	25.756	1.00	32.70
ATOM	375	C	GLU	A	350	33.640	16.687	24.654	1.00	24.52
ATOM	376	O	GLU	A	350	32.596	16.237	24.195	1.00	25.09
ATOM	377	N	VAL	A	351	33.709	17.268	25.847	1.00	22.09
ATOM	378	CA	VAL	A	351	32.513	17.457	26.645	1.00	20.23
ATOM	379	CB	VAL	A	351	32.854	17.885	28.107	1.00	20.75
ATOM	380	CG1	VAL	A	351	31.583	18.062	28.911	1.00	19.11
ATOM	381	CG2	VAL	A	351	33.778	16.851	28.759	1.00	24.36
ATOM	382	C	VAL	A	351	31.625	18.521	25.990	1.00	20.47
ATOM	383	O	VAL	A	351	30.405	18.343	25.878	1.00	21.64
ATOM	384	N	MET	A	352	32.211	19.646	25.592	1.00	23.84
ATOM	385	CA	MET	A	352	31.414	20.705	24.952	1.00	23.93
ATOM	386	CB	MET	A	352	32.235	22.008	24.824	1.00	28.98
ATOM	387	CG	MET	A	352	31.437	23.318	24.552	1.00	26.03
ATOM	388	SD	MET	A	352	30.054	23.586	25.661	1.00	27.59
ATOM	389	CE	MET	A	352	29.087	24.826	24.802	1.00	28.37
ATOM	390	C	MET	A	352	30.897	20.191	23.580	1.00	21.58
ATOM	391	O	MET	A	352	29.743	20.392	23.241	1.00	23.25
ATOM	392	N	TRP	A	353	31.714	19.450	22.847	1.00	20.93
ATOM	393	CA	TRP	A	353	31.249	18.904	21.567	1.00	22.11

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ATOM	394	CB	TRP	A	353	32.375	18.137	20.884	1.00	23.30
ATOM	395	CG	TRP	A	353	33.205	18.935	19.922	1.00	29.85
ATOM	396	CD2	TRP	A	353	33.052	18.969	18.489	1.00	29.97
ATOM	397	CE2	TRP	A	353	34.093	19.776	17.974	1.00	30.39
ATOM	398	CE3	TRP	A	353	32.135	18.385	17.592	1.00	30.52
ATOM	399	CD1	TRP	A	353	34.298	19.711	20.209	1.00	30.84
ATOM	400	NE1	TRP	A	353	34.838	20.216	19.038	1.00	32.97
ATOM	401	CZ2	TRP	A	353	34.248	20.015	16.599	1.00	32.23
ATOM	402	CZ3	TRP	A	353	32.291	18.623	16.228	1.00	29.92
ATOM	403	CH2	TRP	A	353	33.344	19.432	15.748	1.00	30.15
ATOM	404	C	TRP	A	353	30.022	17.992	21.733	1.00	19.54
ATOM	405	O	TRP	A	353	29.027	18.132	21.014	1.00	21.17
ATOM	406	N	GLN	A	354	30.059	17.088	22.714	1.00	20.89
ATOM	407	CA	GLN	A	354	28.938	16.158	22.939	1.00	19.30
ATOM	408	CB	GLN	A	354	29.263	15.167	24.077	1.00	23.50
ATOM	409	CG	GLN	A	354	28.393	13.888	24.093	1.00	24.75
ATOM	410	CD	GLN	A	354	27.436	13.788	25.282	1.00	23.74
ATOM	411	OE1	GLN	A	354	27.297	14.737	26.049	1.00	29.52
ATOM	412	NE2	GLN	A	354	26.767	12.629	25.427	1.00	20.53
ATOM	413	C	GLN	A	354	27.647	16.875	23.248	1.00	16.93
ATOM	414	O	GLN	A	354	26.566	16.516	22.759	1.00	16.41
ATOM	415	N	LEU	A	355	27.747	17.885	24.098	1.00	19.29
ATOM	416	CA	LEU	A	355	26.574	18.645	24.468	1.00	15.90
ATOM	417	CB	LEU	A	355	26.913	19.657	25.579	1.00	15.22
ATOM	418	CG	LEU	A	355	25.802	20.622	25.993	1.00	17.93
ATOM	419	CD1	LEU	A	355	24.582	19.962	26.610	1.00	14.68
ATOM	420	CD2	LEU	A	355	26.418	21.667	26.918	1.00	21.31
ATOM	421	C	LEU	A	355	25.993	19.357	23.240	1.00	11.91
ATOM	422	O	LEU	A	355	24.790	19.348	23.054	1.00	14.23
ATOM	423	N	CYS	A	356	26.827	20.005	22.441	1.00	16.77
ATOM	424	CA	CYS	A	356	26.307	20.691	21.244	1.00	22.19
ATOM	425	CB	CYS	A	356	27.436	21.450	20.561	1.00	21.05
ATOM	426	SG	CYS	A	356	28.067	22.797	21.523	1.00	23.18
ATOM	427	C	CYS	A	356	25.640	19.676	20.263	1.00	21.08
ATOM	428	O	CYS	A	356	24.584	19.943	19.679	1.00	22.09
ATOM	429	N	ALA	A	357	26.228	18.483	20.160	1.00	22.51
ATOM	430	CA	ALA	A	357	25.678	17.449	19.304	1.00	19.05
ATOM	431	CB	ALA	A	357	26.606	16.267	19.264	1.00	25.06
ATOM	432	C	ALA	A	357	24.296	17.048	19.778	1.00	20.99
ATOM	433	O	ALA	A	357	23.387	16.919	18.975	1.00	21.56
ATOM	434	N	ILE	A	358	24.104	16.887	21.092	1.00	21.52
ATOM	435	CA	ILE	A	358	22.782	16.522	21.627	1.00	19.00
ATOM	436	CB	ILE	A	358	22.812	16.382	23.202	1.00	19.36
ATOM	437	CG2	ILE	A	358	21.374	16.383	23.779	1.00	15.59
ATOM	438	CG1	ILE	A	358	23.623	15.153	23.614	1.00	22.16
ATOM	439	CD1	ILE	A	358	24.073	15.174	25.079	1.00	23.75
ATOM	440	C	ILE	A	358	21.747	17.597	21.291	1.00	18.17
ATOM	441	O	ILE	A	358	20.590	17.322	20.947	1.00	17.46
ATOM	442	N	LYS	A	359	22.171	18.843	21.443	1.00	22.77
ATOM	443	CA	LYS	A	359	21.291	19.983	21.206	1.00	21.40
ATOM	444	CB	LYS	A	359	21.931	21.234	21.809	1.00	23.15
ATOM	445	CG	LYS	A	359	22.175	21.133	23.334	1.00	24.28
ATOM	446	CD	LYS	A	359	20.879	20.855	24.063	1.00	24.08
ATOM	447	CE	LYS	A	359	21.061	20.872	25.562	1.00	31.76
ATOM	448	NZ	LYS	A	359	19.730	20.695	26.175	1.00	29.13
ATOM	449	C	LYS	A	359	20.925	20.166	19.721	1.00	16.10
ATOM	450	O	LYS	A	359	19.764	20.377	19.403	1.00	20.28
ATOM	451	N	ILE	A	360	21.914	20.094	18.841	1.00	15.62
ATOM	452	CA	ILE	A	360	21.666	20.199	17.402	1.00	18.38
ATOM	453	CB	ILE	A	360	22.959	19.988	16.595	1.00	24.95
ATOM	454	CG2	ILE	A	360	22.659	19.672	15.136	1.00	28.87
ATOM	455	CG1	ILE	A	360	23.846	21.221	16.659	1.00	25.71
ATOM	456	CD1	ILE	A	360	25.260	20.940	16.214	1.00	28.76
ATOM	457	C	ILE	A	360	20.707	19.085	17.026	1.00	16.86
ATOM	458	O	ILE	A	360	19.678	19.341	16.433	1.00	23.45
ATOM	459	N	THR	A	361	20.986	17.861	17.467	1.00	17.32

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ATOM	460	CA	THR	A	361	20.131	16.724	17.118	1.00	17.15
ATOM	461	CB	THR	A	361	20.647	15.411	17.703	1.00	21.09
ATOM	462	OG1	THR	A	361	22.030	15.263	17.385	1.00	21.21
ATOM	463	CG2	THR	A	361	19.842	14.207	17.146	1.00	23.13
ATOM	464	C	THR	A	361	18.687	16.887	17.514	1.00	22.12
ATOM	465	O	THR	A	361	17.786	16.414	16.813	1.00	22.98
ATOM	466	N	GLU	A	362	18.455	17.530	18.660	1.00	22.63
ATOM	467	CA	GLU	A	362	17.092	17.761	19.121	1.00	21.83
ATOM	468	CB	GLU	A	362	17.076	18.335	20.541	1.00	25.44
ATOM	469	CG	GLU	A	362	15.729	18.156	21.228	1.00	45.77
ATOM	470	CD	GLU	A	362	15.382	19.260	22.253	1.00	61.04
ATOM	471	OE1	GLU	A	362	16.281	19.648	23.059	1.00	67.71
ATOM	472	OE2	GLU	A	362	14.199	19.723	22.249	1.00	58.48
ATOM	473	C	GLU	A	362	16.407	18.717	18.137	1.00	17.52
ATOM	474	O	GLU	A	362	15.226	18.567	17.836	1.00	18.31
ATOM	475	N	ALA	A	363	17.148	19.711	17.656	1.00	17.89
ATOM	476	CA	ALA	A	363	16.613	20.652	16.656	1.00	22.83
ATOM	477	CB	ALA	A	363	17.624	21.753	16.358	1.00	21.95
ATOM	478	C	ALA	A	363	16.304	19.896	15.348	1.00	21.89
ATOM	479	O	ALA	A	363	15.286	20.140	14.706	1.00	24.25
ATOM	480	N	ILE	A	364	17.196	18.994	14.952	1.00	23.12
ATOM	481	CA	ILE	A	364	16.995	18.214	13.715	1.00	23.74
ATOM	482	CB	ILE	A	364	18.255	17.379	13.357	1.00	20.60
ATOM	483	CG2	ILE	A	364	17.943	16.320	12.288	1.00	20.36
ATOM	484	CG1	ILE	A	364	19.349	18.329	12.855	1.00	16.57
ATOM	485	CD1	ILE	A	364	20.748	17.766	12.820	1.00	17.77
ATOM	486	C	ILE	A	364	15.709	17.382	13.705	1.00	28.19
ATOM	487	O	ILE	A	364	14.969	17.380	12.715	1.00	29.54
ATOM	488	N	GLN	A	365	15.370	16.784	14.842	1.00	28.50
ATOM	489	CA	GLN	A	365	14.159	15.976	14.937	1.00	28.61
ATOM	490	CB	GLN	A	365	14.049	15.352	16.309	1.00	34.56
ATOM	491	CG	GLN	A	365	15.324	14.645	16.719	1.00	46.55
ATOM	492	CD	GLN	A	365	15.071	13.640	17.800	1.00	53.78
ATOM	493	OE1	GLN	A	365	13.968	13.106	17.901	1.00	64.74
ATOM	494	NE2	GLN	A	365	16.077	13.366	18.617	1.00	55.00
ATOM	495	C	GLN	A	365	12.893	16.737	14.620	1.00	26.94
ATOM	496	O	GLN	A	365	11.919	16.145	14.172	1.00	30.81
ATOM	497	N	TYR	A	366	12.884	18.036	14.903	1.00	26.99
ATOM	498	CA	TYR	A	366	11.733	18.889	14.598	1.00	23.20
ATOM	499	CB	TYR	A	366	11.822	20.212	15.376	1.00	25.77
ATOM	500	CG	TYR	A	366	11.345	20.112	16.816	1.00	27.13
ATOM	501	CD1	TYR	A	366	12.246	20.050	17.880	1.00	27.24
ATOM	502	CE1	TYR	A	366	11.787	19.956	19.198	1.00	32.73
ATOM	503	CD2	TYR	A	366	9.984	20.075	17.103	1.00	29.26
ATOM	504	CE2	TYR	A	366	9.521	19.976	18.402	1.00	33.96
ATOM	505	CZ	TYR	A	366	10.420	19.917	19.445	1.00	36.94
ATOM	506	OH	TYR	A	366	9.925	19.808	20.729	1.00	45.77
ATOM	507	C	TYR	A	366	11.743	19.165	13.084	1.00	22.71
ATOM	508	O	TYR	A	366	10.688	19.258	12.450	1.00	21.29
ATOM	509	N	VAL	A	367	12.948	19.314	12.527	1.00	23.15
ATOM	510	CA	VAL	A	367	13.130	19.536	11.085	1.00	25.23
ATOM	511	CB	VAL	A	367	14.586	19.907	10.742	1.00	22.53
ATOM	512	CG1	VAL	A	367	14.798	19.914	9.224	1.00	20.69
ATOM	513	CG2	VAL	A	367	14.878	21.280	11.292	1.00	17.32
ATOM	514	C	VAL	A	367	12.650	18.303	10.281	1.00	28.13
ATOM	515	O	VAL	A	367	12.027	18.449	9.236	1.00	28.63
ATOM	516	N	VAL	A	368	12.929	17.098	10.771	1.00	27.16
ATOM	517	CA	VAL	A	368	12.450	15.890	10.116	1.00	27.59
ATOM	518	CB	VAL	A	368	13.048	14.606	10.759	1.00	23.81
ATOM	519	CG1	VAL	A	368	12.340	13.380	10.226	1.00	29.32
ATOM	520	CG2	VAL	A	368	14.550	14.505	10.469	1.00	18.99
ATOM	521	C	VAL	A	368	10.894	15.861	10.144	1.00	32.37
ATOM	522	O	VAL	A	368	10.268	15.429	9.159	1.00	33.74
ATOM	523	N	GLU	A	369	10.268	16.324	11.242	1.00	26.37
ATOM	524	CA	GLU	A	369	8.801	16.364	11.318	1.00	26.23
ATOM	525	CB	GLU	A	369	8.281	16.756	12.712	1.00	29.58

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ATOM	526	CG	GLU	A	369	8.304	15.647	13.763	1.00	33.78
ATOM	527	CD	GLU	A	369	7.736	14.303	13.284	1.00	34.63
ATOM	528	OE1	GLU	A	369	6.610	14.253	12.741	1.00	36.64
ATOM	529	OE2	GLU	A	369	8.430	13.280	13.476	1.00	40.81
ATOM	530	C	GLU	A	369	8.269	17.358	10.291	1.00	26.20
ATOM	531	O	GLU	A	369	7.213	17.143	9.713	1.00	29.54
ATOM	532	N	PHE	A	370	8.970	18.476	10.118	1.00	24.75
ATOM	533	CA	PHE	A	370	8.607	19.475	9.114	1.00	24.70
ATOM	534	CB	PHE	A	370	9.615	20.615	9.162	1.00	23.84
ATOM	535	CG	PHE	A	370	9.415	21.663	8.093	1.00	24.23
ATOM	536	CD1	PHE	A	370	8.265	22.444	8.071	1.00	24.20
ATOM	537	CD2	PHE	A	370	10.415	21.918	7.161	1.00	24.12
ATOM	538	CE1	PHE	A	370	8.120	23.468	7.150	1.00	27.38
ATOM	539	CE2	PHE	A	370	10.276	22.943	6.234	1.00	26.73
ATOM	540	CZ	PHE	A	370	9.125	23.722	6.231	1.00	24.57
ATOM	541	C	PHE	A	370	8.648	18.805	7.712	1.00	26.16
ATOM	542	O	PHE	A	370	7.666	18.841	6.966	1.00	24.95
ATOM	543	N	ALA	A	371	9.780	18.172	7.395	1.00	25.24
ATOM	544	CA	ALA	A	371	9.988	17.459	6.130	1.00	31.38
ATOM	545	CB	ALA	A	371	11.281	16.681	6.171	1.00	27.13
ATOM	546	C	ALA	A	371	8.829	16.525	5.794	1.00	33.49
ATOM	547	O	ALA	A	371	8.328	16.550	4.674	1.00	35.75
ATOM	548	N	LYS	A	372	8.380	15.730	6.766	1.00	32.11
ATOM	549	CA	LYS	A	372	7.260	14.817	6.547	1.00	32.07
ATOM	550	CB	LYS	A	372	7.025	13.969	7.780	1.00	31.18
ATOM	551	CG	LYS	A	372	8.142	13.030	8.132	1.00	34.27
ATOM	552	CD	LYS	A	372	7.714	12.198	9.322	1.00	41.43
ATOM	553	CE	LYS	A	372	8.898	11.535	9.996	1.00	47.18
ATOM	554	NZ	LYS	A	372	8.490	10.731	11.203	1.00	52.21
ATOM	555	C	LYS	A	372	5.920	15.464	6.175	1.00	36.43
ATOM	556	O	LYS	A	372	5.047	14.804	5.612	1.00	39.27
ATOM	557	N	ARG	A	373	5.742	16.735	6.511	1.00	38.37
ATOM	558	CA	ARG	A	373	4.484	17.435	6.242	1.00	40.66
ATOM	559	CB	ARG	A	373	4.201	18.447	7.355	1.00	45.55
ATOM	560	CG	ARG	A	373	4.681	18.002	8.714	1.00	54.93
ATOM	561	CD	ARG	A	373	3.682	17.131	9.441	1.00	59.22
ATOM	562	NE	ARG	A	373	2.817	17.960	10.278	1.00	65.72
ATOM	563	CZ	ARG	A	373	2.860	17.988	11.607	1.00	63.53
ATOM	564	NH1	ARG	A	373	3.723	17.222	12.261	1.00	61.86
ATOM	565	NH2	ARG	A	373	2.057	18.802	12.281	1.00	66.65
ATOM	566	C	ARG	A	373	4.503	18.179	4.916	1.00	41.35
ATOM	567	O	ARG	A	373	3.496	18.773	4.516	1.00	40.31
ATOM	568	N	ILE	A	374	5.669	18.203	4.271	1.00	41.14
ATOM	569	CA	ILE	A	374	5.806	18.883	2.996	1.00	40.72
ATOM	570	CB	ILE	A	374	7.237	19.329	2.697	1.00	36.14
ATOM	571	CG2	ILE	A	374	7.298	19.939	1.299	1.00	32.36
ATOM	572	CG1	ILE	A	374	7.675	20.387	3.702	1.00	34.12
ATOM	573	CD1	ILE	A	374	9.159	20.603	3.712	1.00	36.75
ATOM	574	C	ILE	A	374	5.302	18.054	1.831	1.00	45.90
ATOM	575	O	ILE	A	374	5.733	16.929	1.583	1.00	42.19
ATOM	576	N	ASP	A	375	4.301	18.625	1.183	1.00	50.81
ATOM	577	CA	ASP	A	375	3.654	18.084	-0.002	1.00	52.36
ATOM	578	CB	ASP	A	375	2.859	19.229	-0.649	1.00	60.93
ATOM	579	CG	ASP	A	375	3.543	20.613	-0.449	1.00	68.87
ATOM	580	OD1	ASP	A	375	4.421	20.987	-1.277	1.00	67.94
ATOM	581	OD2	ASP	A	375	3.225	21.301	0.561	1.00	63.03
ATOM	582	C	ASP	A	375	4.690	17.547	-0.998	1.00	48.88
ATOM	583	O	ASP	A	375	5.454	18.309	-1.595	1.00	48.00
ATOM	584	N	GLY	A	376	4.743	16.234	-1.152	1.00	45.67
ATOM	585	CA	GLY	A	376	5.683	15.669	-2.103	1.00	43.48
ATOM	586	C	GLY	A	376	6.816	14.872	-1.514	1.00	40.36
ATOM	587	O	GLY	A	376	7.200	13.837	-2.052	1.00	38.28
ATOM	588	N	PHE	A	377	7.339	15.346	-0.394	1.00	37.97
ATOM	589	CA	PHE	A	377	8.448	14.677	0.270	1.00	34.67
ATOM	590	CB	PHE	A	377	8.826	15.430	1.567	1.00	34.08
ATOM	591	CG	PHE	A	377	10.054	14.887	2.245	1.00	29.16



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ATOM	592	CD1	PHE	A	377	11.305	15.422	1.962	1.00	27.28
ATOM	593	CD2	PHE	A	377	9.964	13.778	3.096	1.00	30.07
ATOM	594	CE1	PHE	A	377	12.453	14.859	2.496	1.00	28.02
ATOM	595	CE2	PHE	A	377	11.095	13.205	3.637	1.00	29.05
ATOM	596	CZ	PHE	A	377	12.353	13.746	3.333	1.00	28.74
ATOM	597	C	PHE	A	377	8.203	13.197	0.572	1.00	34.90
ATOM	598	O	PHE	A	377	9.076	12.361	0.305	1.00	35.66
ATOM	599	N	MET	A	378	7.060	12.871	1.169	1.00	34.38
ATOM	600	CA	MET	A	378	6.766	11.491	1.512	1.00	38.67
ATOM	601	CB	MET	A	378	5.565	11.393	2.457	1.00	41.83
ATOM	602	CG	MET	A	378	5.882	11.754	3.909	1.00	48.90
ATOM	603	SD	MET	A	378	7.422	10.982	4.496	1.00	56.77
ATOM	604	CE	MET	A	378	6.884	9.291	4.787	1.00	57.67
ATOM	605	C	MET	A	378	6.574	10.586	0.301	1.00	42.95
ATOM	606	O	MET	A	378	6.564	9.363	0.428	1.00	43.36
ATOM	607	N	GLU	A	379	6.427	11.184	-0.877	1.00	44.95
ATOM	608	CA	GLU	A	379	6.248	10.399	-2.086	1.00	45.80
ATOM	609	CB	GLU	A	379	5.359	11.144	-3.071	1.00	52.39
ATOM	610	CG	GLU	A	379	3.943	11.354	-2.587	1.00	61.32
ATOM	611	CD	GLU	A	379	3.127	12.219	-3.537	1.00	71.44
ATOM	612	OE1	GLU	A	379	3.681	13.182	-4.126	1.00	73.32
ATOM	613	OE2	GLU	A	379	1.920	11.933	-3.693	1.00	77.96
ATOM	614	C	GLU	A	379	7.581	10.057	-2.741	1.00	43.64
ATOM	615	O	GLU	A	379	7.655	9.144	-3.553	1.00	43.83
ATOM	616	N	LEU	A	380	8.633	10.794	-2.409	1.00	40.33
ATOM	617	CA	LEU	A	380	9.939	10.521	-2.986	1.00	40.49
ATOM	618	CB	LEU	A	380	10.949	11.562	-2.536	1.00	39.57
ATOM	619	CG	LEU	A	380	10.996	12.909	-3.242	1.00	43.35
ATOM	620	CD1	LEU	A	380	9.660	13.313	-3.786	1.00	48.51
ATOM	621	CD2	LEU	A	380	11.496	13.947	-2.266	1.00	43.53
ATOM	622	C	LEU	A	380	10.374	9.151	-2.509	1.00	43.17
ATOM	623	O	LEU	A	380	9.702	8.546	-1.675	1.00	41.79
ATOM	624	N	CYS	A	381	11.480	8.650	-3.053	1.00	46.89
ATOM	625	CA	CYS	A	381	11.988	7.339	-2.651	1.00	51.11
ATOM	626	CB	CYS	A	381	12.676	6.632	-3.838	1.00	48.63
ATOM	627	SG	CYS	A	381	14.146	7.457	-4.487	1.00	48.71
ATOM	628	C	CYS	A	381	12.938	7.479	-1.437	1.00	53.70
ATOM	629	O	CYS	A	381	13.731	8.427	-1.357	1.00	54.89
ATOM	630	N	GLN	A	382	12.813	6.559	-0.478	1.00	56.40
ATOM	631	CA	GLN	A	382	13.625	6.552	0.747	1.00	57.37
ATOM	632	CB	GLN	A	382	13.717	5.125	1.299	1.00	66.42
ATOM	633	CG	GLN	A	382	14.527	4.981	2.596	1.00	80.23
ATOM	634	CD	GLN	A	382	14.924	3.529	2.908	1.00	87.56
ATOM	635	OE1	GLN	A	382	14.364	2.579	2.351	1.00	93.99
ATOM	636	NE2	GLN	A	382	15.916	3.361	3.781	1.00	90.30
ATOM	637	C	GLN	A	382	15.030	7.108	0.529	1.00	52.28
ATOM	638	O	GLN	A	382	15.534	7.891	1.315	1.00	52.44
ATOM	639	N	ASN	A	383	15.644	6.716	-0.571	1.00	48.24
ATOM	640	CA	ASN	A	383	16.975	7.166	-0.891	1.00	46.79
ATOM	641	CB	ASN	A	383	17.393	6.604	-2.241	1.00	55.14
ATOM	642	CG	ASN	A	383	17.496	5.100	-2.232	1.00	63.92
ATOM	643	OD1	ASN	A	383	18.603	4.559	-2.272	1.00	68.19
ATOM	644	ND2	ASN	A	383	16.350	4.405	-2.198	1.00	65.25
ATOM	645	C	ASN	A	383	17.000	8.669	-0.986	1.00	42.13
ATOM	646	O	ASN	A	383	17.853	9.331	-0.408	1.00	38.96
ATOM	647	N	ASP	A	384	16.064	9.203	-1.749	1.00	35.42
ATOM	648	CA	ASP	A	384	16.015	10.633	-1.945	1.00	35.36
ATOM	649	CB	ASP	A	384	15.137	10.984	-3.146	1.00	35.18
ATOM	650	CG	ASP	A	384	15.790	10.618	-4.491	1.00	36.49
ATOM	651	OD1	ASP	A	384	16.835	9.919	-4.525	1.00	35.12
ATOM	652	OD2	ASP	A	384	15.245	11.049	-5.519	1.00	34.59
ATOM	653	C	ASP	A	384	15.578	11.376	-0.701	1.00	30.33
ATOM	654	O	ASP	A	384	15.999	12.501	-0.484	1.00	27.59
ATOM	655	N	GLN	A	385	14.713	10.760	0.098	1.00	31.50
ATOM	656	CA	GLN	A	385	14.280	11.403	1.348	1.00	33.11
ATOM	657	CB	GLN	A	385	13.215	10.577	2.033	1.00	28.85

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ATOM	658	CG	GLN	A	385	11.932	10.516	1.281	1.00	29.25
ATOM	659	CD	GLN	A	385	10.981	9.578	1.942	1.00	35.13
ATOM	660	OE1	GLN	A	385	11.392	8.704	2.711	1.00	39.80
ATOM	661	NE2	GLN	A	385	9.703	9.737	1.663	1.00	34.78
ATOM	662	C	GLN	A	385	15.488	11.552	2.277	1.00	31.53
ATOM	663	O	GLN	A	385	15.751	12.632	2.816	1.00	29.68
ATOM	664	N	ILE	A	386	16.251	10.466	2.394	1.00	29.20
ATOM	665	CA	ILE	A	386	17.452	10.430	3.208	1.00	31.16
ATOM	666	CB	ILE	A	386	17.992	8.987	3.310	1.00	30.97
ATOM	667	CG2	ILE	A	386	19.411	8.959	3.925	1.00	29.51
ATOM	668	CG1	ILE	A	386	16.982	8.148	4.103	1.00	31.82
ATOM	669	CD1	ILE	A	386	17.452	6.761	4.458	1.00	39.13
ATOM	670	C	ILE	A	386	18.518	11.411	2.696	1.00	30.95
ATOM	671	O	ILE	A	386	19.068	12.189	3.473	1.00	31.12
ATOM	672	N	VAL	A	387	18.788	11.400	1.392	1.00	30.52
ATOM	673	CA	VAL	A	387	19.771	12.314	0.800	1.00	26.90
ATOM	674	CB	VAL	A	387	19.877	12.122	-0.763	1.00	25.37
ATOM	675	CG1	VAL	A	387	20.555	13.328	-1.412	1.00	20.02
ATOM	676	CG2	VAL	A	387	20.658	10.864	-1.088	1.00	22.89
ATOM	677	C	VAL	A	387	19.394	13.786	1.104	1.00	28.03
ATOM	678	O	VAL	A	387	20.265	14.602	1.446	1.00	27.40
ATOM	679	N	LEU	A	388	18.099	14.114	0.975	1.00	27.01
ATOM	680	CA	LEU	A	388	17.606	15.482	1.212	1.00	25.83
ATOM	681	CB	LEU	A	388	16.149	15.631	0.776	1.00	25.27
ATOM	682	CG	LEU	A	388	15.822	15.597	-0.723	1.00	23.66
ATOM	683	CD1	LEU	A	388	14.344	15.786	-0.898	1.00	24.29
ATOM	684	CD2	LEU	A	388	16.587	16.686	-1.461	1.00	27.16
ATOM	685	C	LEU	A	388	17.738	15.871	2.683	1.00	26.40
ATOM	686	O	LEU	A	388	18.094	16.998	2.998	1.00	25.91
ATOM	687	N	LEU	A	389	17.461	14.928	3.572	1.00	25.45
ATOM	688	CA	LEU	A	389	17.578	15.192	4.994	1.00	23.81
ATOM	689	CB	LEU	A	389	16.915	14.096	5.803	1.00	23.38
ATOM	690	CG	LEU	A	389	15.402	14.206	5.789	1.00	22.32
ATOM	691	CD1	LEU	A	389	14.785	13.003	6.476	1.00	25.13
ATOM	692	CD2	LEU	A	389	14.984	15.501	6.427	1.00	19.09
ATOM	693	C	LEU	A	389	19.020	15.299	5.376	1.00	21.15
ATOM	694	O	LEU	A	389	19.410	16.257	6.028	1.00	26.81
ATOM	695	N	LYS	A	390	19.849	14.373	4.916	1.00	18.69
ATOM	696	CA	LYS	A	390	21.250	14.429	5.273	1.00	21.34
ATOM	697	CB	LYS	A	390	22.050	13.326	4.592	1.00	24.41
ATOM	698	CG	LYS	A	390	21.938	11.960	5.200	1.00	29.06
ATOM	699	CD	LYS	A	390	23.067	11.081	4.673	1.00	31.45
ATOM	700	CE	LYS	A	390	23.062	9.718	5.342	1.00	40.63
ATOM	701	NZ	LYS	A	390	24.240	8.890	4.933	1.00	46.61
ATOM	702	C	LYS	A	390	21.884	15.751	4.907	1.00	25.73
ATOM	703	O	LYS	A	390	22.706	16.287	5.644	1.00	26.32
ATOM	704	N	ALA	A	391	21.478	16.295	3.770	1.00	25.48
ATOM	705	CA	ALA	A	391	22.065	17.527	3.281	1.00	23.46
ATOM	706	CB	ALA	A	391	22.076	17.505	1.766	1.00	26.48
ATOM	707	C	ALA	A	391	21.401	18.795	3.750	1.00	20.95
ATOM	708	O	ALA	A	391	22.074	19.789	4.005	1.00	27.25
ATOM	709	N	GLY	A	392	20.082	18.773	3.838	1.00	21.07
ATOM	710	CA	GLY	A	392	19.349	19.965	4.202	1.00	22.76
ATOM	711	C	GLY	A	392	18.923	20.133	5.638	1.00	23.17
ATOM	712	O	GLY	A	392	18.420	21.184	5.972	1.00	20.90
ATOM	713	N	SER	A	393	19.087	19.105	6.471	1.00	23.99
ATOM	714	CA	SER	A	393	18.706	19.178	7.889	1.00	23.62
ATOM	715	CB	SER	A	393	19.056	17.874	8.593	1.00	20.71
ATOM	716	OG	SER	A	393	17.926	17.045	8.510	1.00	31.96
ATOM	717	C	SER	A	393	19.343	20.322	8.656	1.00	17.30
ATOM	718	O	SER	A	393	18.645	21.149	9.223	1.00	19.88
ATOM	719	N	LEU	A	394	20.670	20.332	8.677	1.00	20.09
ATOM	720	CA	LEU	A	394	21.442	21.348	9.365	1.00	21.08
ATOM	721	CB	LEU	A	394	22.940	21.032	9.274	1.00	19.93
ATOM	722	CG	LEU	A	394	23.831	20.918	10.516	1.00	26.08
ATOM	723	CD1	LEU	A	394	25.207	21.380	10.158	1.00	21.54

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ATOM	724	CD2	LEU	A	394	23.285	21.730	11.705	1.00	22.96
ATOM	725	C	LEU	A	394	21.161	22.713	8.753	1.00	23.43
ATOM	726	O	LEU	A	394	21.132	23.717	9.462	1.00	21.36
ATOM	727	N	GLU	A	395	20.942	22.759	7.436	1.00	22.13
ATOM	728	CA	GLU	A	395	20.642	24.037	6.787	1.00	20.91
ATOM	729	CB	GLU	A	395	20.574	23.890	5.260	1.00	22.76
ATOM	730	CG	GLU	A	395	21.881	23.459	4.611	1.00	23.62
ATOM	731	CD	GLU	A	395	21.809	23.461	3.084	1.00	26.69
ATOM	732	OE1	GLU	A	395	22.852	23.482	2.434	1.00	27.60
ATOM	733	OE2	GLU	A	395	20.709	23.428	2.526	1.00	22.32
ATOM	734	C	GLU	A	395	19.342	24.632	7.318	1.00	18.31
ATOM	735	O	GLU	A	395	19.270	25.832	7.574	1.00	20.03
ATOM	736	N	VAL	A	396	18.311	23.810	7.498	1.00	18.03
ATOM	737	CA	VAL	A	396	17.043	24.331	8.031	1.00	24.17
ATOM	738	CB	VAL	A	396	15.891	23.342	7.818	1.00	20.05
ATOM	739	CG1	VAL	A	396	14.587	23.854	8.517	1.00	18.41
ATOM	740	CG2	VAL	A	396	15.663	23.177	6.288	1.00	22.83
ATOM	741	C	VAL	A	396	17.174	24.744	9.525	1.00	25.12
ATOM	742	O	VAL	A	396	16.476	25.639	10.006	1.00	26.40
ATOM	743	N	VAL	A	397	18.077	24.073	10.232	1.00	23.34
ATOM	744	CA	VAL	A	397	18.358	24.401	11.617	1.00	18.37
ATOM	745	CB	VAL	A	397	19.296	23.338	12.232	1.00	19.79
ATOM	746	CG1	VAL	A	397	19.915	23.829	13.534	1.00	20.93
ATOM	747	CG2	VAL	A	397	18.517	22.069	12.472	1.00	16.14
ATOM	748	C	VAL	A	397	19.006	25.802	11.635	1.00	17.79
ATOM	749	O	VAL	A	397	18.547	26.676	12.359	1.00	21.81
ATOM	750	N	PHE	A	398	19.981	26.058	10.760	1.00	16.57
ATOM	751	CA	PHE	A	398	20.625	27.355	10.735	1.00	12.50
ATOM	752	CB	PHE	A	398	21.910	27.288	9.955	1.00	16.85
ATOM	753	CG	PHE	A	398	23.017	26.588	10.669	1.00	22.50
ATOM	754	CD1	PHE	A	398	23.316	26.899	11.986	1.00	21.63
ATOM	755	CD2	PHE	A	398	23.796	25.645	10.014	1.00	21.83
ATOM	756	CE1	PHE	A	398	24.375	26.279	12.623	1.00	22.54
ATOM	757	CE2	PHE	A	398	24.859	25.021	10.652	1.00	23.29
ATOM	758	CZ	PHE	A	398	25.151	25.334	11.953	1.00	22.58
ATOM	759	C	PHE	A	398	19.718	28.486	10.249	1.00	19.24
ATOM	760	O	PHE	A	398	19.944	29.669	10.570	1.00	19.14
ATOM	761	N	ILE	A	399	18.663	28.138	9.513	1.00	20.43
ATOM	762	CA	ILE	A	399	17.685	29.145	9.077	1.00	21.75
ATOM	763	CB	ILE	A	399	16.790	28.652	7.848	1.00	23.69
ATOM	764	CG2	ILE	A	399	15.574	29.562	7.656	1.00	17.51
ATOM	765	CG1	ILE	A	399	17.608	28.583	6.538	1.00	26.64
ATOM	766	CD1	ILE	A	399	16.942	27.745	5.397	1.00	17.97
ATOM	767	C	ILE	A	399	16.771	29.382	10.296	1.00	18.17
ATOM	768	O	ILE	A	399	16.484	30.507	10.662	1.00	20.59
ATOM	769	N	ARG	A	400	16.317	28.307	10.921	1.00	19.22
ATOM	770	CA	ARG	A	400	15.451	28.415	12.087	1.00	20.62
ATOM	771	CB	ARG	A	400	15.000	27.029	12.553	1.00	17.24
ATOM	772	CG	ARG	A	400	13.783	26.537	11.852	1.00	15.74
ATOM	773	CD	ARG	A	400	13.420	25.143	12.246	1.00	17.01
ATOM	774	NE	ARG	A	400	12.189	24.760	11.553	1.00	21.84
ATOM	775	CZ	ARG	A	400	11.371	23.775	11.909	1.00	21.38
ATOM	776	NH1	ARG	A	400	11.643	23.021	12.976	1.00	27.51
ATOM	777	NH2	ARG	A	400	10.221	23.610	11.261	1.00	19.58
ATOM	778	C	ARG	A	400	16.132	29.177	13.235	1.00	22.12
ATOM	779	O	ARG	A	400	15.456	29.834	14.016	1.00	22.87
ATOM	780	N	MET	A	401	17.462	29.140	13.283	1.00	20.39
ATOM	781	CA	MET	A	401	18.251	29.813	14.320	1.00	22.78
ATOM	782	CB	MET	A	401	19.740	29.612	14.026	1.00	21.38
ATOM	783	CG	MET	A	401	20.681	30.082	15.096	1.00	17.22
ATOM	784	SD	MET	A	401	22.356	30.190	14.524	1.00	24.87
ATOM	785	CE	MET	A	401	22.858	28.674	14.579	1.00	30.52
ATOM	786	C	MET	A	401	17.942	31.308	14.448	1.00	27.16
ATOM	787	O	MET	A	401	18.177	31.913	15.495	1.00	24.54
ATOM	788	N	CYS	A	402	17.451	31.901	13.362	1.00	28.58
ATOM	789	CA	CYS	A	402	17.102	33.327	13.340	1.00	33.94

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ATOM	790	CB	CYS	A	402	16.827	33.801	11.911	1.00	34.97
ATOM	791	SG	CYS	A	402	18.382	33.864	11.142	1.00	54.57
ATOM	792	C	CYS	A	402	15.947	33.699	14.236	1.00	33.06
ATOM	793	O	CYS	A	402	15.871	34.838	14.722	1.00	36.03
ATOM	794	N	ARG	A	403	15.033	32.759	14.438	1.00	30.48
ATOM	795	CA	ARG	A	403	13.903	33.013	15.316	1.00	30.17
ATOM	796	CB	ARG	A	403	12.846	31.936	15.165	1.00	27.27
ATOM	797	CG	ARG	A	403	12.529	31.529	13.760	1.00	32.18
ATOM	798	CD	ARG	A	403	11.217	30.784	13.777	1.00	32.00
ATOM	799	NE	ARG	A	403	11.202	29.740	14.794	1.00	37.42
ATOM	800	CZ	ARG	A	403	10.188	29.482	15.616	1.00	33.92
ATOM	801	NH1	ARG	A	403	9.078	30.195	15.575	1.00	34.55
ATOM	802	NH2	ARG	A	403	10.257	28.436	16.428	1.00	42.16
ATOM	803	C	ARG	A	403	14.368	32.993	16.780	1.00	29.68
ATOM	804	O	ARG	A	403	13.653	33.472	17.649	1.00	30.31
ATOM	805	N	ALA	A	404	15.556	32.431	17.016	1.00	26.70
ATOM	806	CA	ALA	A	404	16.145	32.267	18.336	1.00	21.83
ATOM	807	CB	ALA	A	404	16.328	30.768	18.612	1.00	17.43
ATOM	808	C	ALA	A	404	17.490	32.962	18.394	1.00	23.99
ATOM	809	O	ALA	A	404	18.371	32.543	19.134	1.00	26.66
ATOM	810	N	PHE	A	405	17.694	33.990	17.573	1.00	26.59
ATOM	811	CA	PHE	A	405	18.977	34.705	17.557	1.00	24.98
ATOM	812	CB	PHE	A	405	19.713	34.470	16.227	1.00	18.47
ATOM	813	CG	PHE	A	405	21.110	35.018	16.187	1.00	17.64
ATOM	814	CD1	PHE	A	405	22.202	34.177	16.313	1.00	16.69
ATOM	815	CD2	PHE	A	405	21.345	36.370	15.956	1.00	19.09
ATOM	816	CE1	PHE	A	405	23.514	34.669	16.199	1.00	21.32
ATOM	817	CE2	PHE	A	405	22.651	36.871	15.841	1.00	17.33
ATOM	818	CZ	PHE	A	405	23.734	36.032	15.957	1.00	19.99
ATOM	819	C	PHE	A	405	18.765	36.197	17.805	1.00	28.98
ATOM	820	O	PHE	A	405	17.845	36.789	17.256	1.00	31.78
ATOM	821	N	ASP	A	406	19.581	36.763	18.703	1.00	31.70
ATOM	822	CA	ASP	A	406	19.556	38.180	19.084	1.00	30.27
ATOM	823	CB	ASP	A	406	19.786	38.339	20.598	1.00	30.55
ATOM	824	CG	ASP	A	406	19.689	39.798	21.081	1.00	34.22
ATOM	825	OD1	ASP	A	406	19.722	40.747	20.278	1.00	31.76
ATOM	826	OD2	ASP	A	406	19.575	40.004	22.299	1.00	33.44
ATOM	827	C	ASP	A	406	20.671	38.897	18.330	1.00	29.96
ATOM	828	O	ASP	A	406	21.821	38.953	18.804	1.00	29.82
ATOM	829	N	SER	A	407	20.302	39.510	17.203	1.00	28.41
ATOM	830	CA	SER	A	407	21.263	40.224	16.374	1.00	34.69
ATOM	831	CB	SER	A	407	20.597	40.719	15.093	1.00	37.05
ATOM	832	OG	SER	A	407	21.531	40.766	14.018	1.00	51.86
ATOM	833	C	SER	A	407	21.922	41.381	17.115	1.00	34.14
ATOM	834	O	SER	A	407	23.147	41.501	17.139	1.00	35.01
ATOM	835	N	GLN	A	408	21.113	42.206	17.764	1.00	38.76
ATOM	836	CA	GLN	A	408	21.632	43.345	18.519	1.00	40.20
ATOM	837	CB	GLN	A	408	20.516	43.981	19.353	1.00	48.77
ATOM	838	CG	GLN	A	408	19.250	44.338	18.577	1.00	63.31
ATOM	839	CD	GLN	A	408	18.001	44.400	19.467	1.00	70.33
ATOM	840	OE1	GLN	A	408	17.761	45.387	20.175	1.00	73.70
ATOM	841	NE2	GLN	A	408	17.185	43.347	19.405	1.00	72.43
ATOM	842	C	GLN	A	408	22.744	42.908	19.463	1.00	36.52
ATOM	843	O	GLN	A	408	23.827	43.493	19.484	1.00	36.77
ATOM	844	N	ASN	A	409	22.514	41.803	20.156	1.00	32.86
ATOM	845	CA	ASN	A	409	23.466	41.338	21.132	1.00	31.16
ATOM	846	CB	ASN	A	409	22.722	41.083	22.438	1.00	34.90
ATOM	847	CG	ASN	A	409	22.115	42.371	23.024	1.00	35.74
ATOM	848	OD1	ASN	A	409	22.850	43.282	23.401	1.00	38.31
ATOM	849	ND2	ASN	A	409	20.784	42.457	23.076	1.00	31.20
ATOM	850	C	ASN	A	409	24.369	40.175	20.752	1.00	32.11
ATOM	851	O	ASN	A	409	25.179	39.729	21.574	1.00	34.18
ATOM	852	N	ASN	A	410	24.291	39.743	19.494	1.00	29.63
ATOM	853	CA	ASN	A	410	25.128	38.646	18.979	1.00	27.78
ATOM	854	CB	ASN	A	410	26.597	39.063	18.877	1.00	24.50
ATOM	855	CG	ASN	A	410	27.360	38.235	17.866	1.00	25.12

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ATOM	856	OD1	ASN	A	410	26.851	37.955	16.780	1.00	29.04
ATOM	857	ND2	ASN	A	410	28.568	37.813	18.224	1.00	27.47
ATOM	858	C	ASN	A	410	25.016	37.476	19.928	1.00	28.72
ATOM	859	O	ASN	A	410	26.016	36.970	20.457	1.00	27.57
ATOM	860	N	THR	A	411	23.813	36.948	20.020	1.00	27.68
ATOM	861	CA	THR	A	411	23.602	35.905	20.977	1.00	26.24
ATOM	862	CB	THR	A	411	23.208	36.681	22.253	1.00	27.76
ATOM	863	OG1	THR	A	411	24.162	36.446	23.305	1.00	31.38
ATOM	864	CG2	THR	A	411	21.784	36.514	22.604	1.00	16.40
ATOM	865	C	THR	A	411	22.577	34.896	20.464	1.00	22.40
ATOM	866	O	THR	A	411	21.649	35.282	19.779	1.00	24.61
ATOM	867	N	VAL	A	412	22.768	33.612	20.771	1.00	20.76
ATOM	868	CA	VAL	A	412	21.857	32.528	20.343	1.00	19.57
ATOM	869	CB	VAL	A	412	22.607	31.487	19.475	1.00	19.83
ATOM	870	CG1	VAL	A	412	21.655	30.780	18.524	1.00	18.01
ATOM	871	CG2	VAL	A	412	23.691	32.130	18.740	1.00	33.67
ATOM	872	C	VAL	A	412	21.278	31.708	21.508	1.00	18.12
ATOM	873	O	VAL	A	412	22.009	31.325	22.411	1.00	23.18
ATOM	874	N	TYR	A	413	19.990	31.386	21.453	1.00	16.25
ATOM	875	CA	TYR	A	413	19.320	30.575	22.465	1.00	17.45
ATOM	876	CB	TYR	A	413	17.855	30.512	22.122	1.00	17.78
ATOM	877	CG	TYR	A	413	16.935	29.951	23.181	1.00	25.60
ATOM	878	CD1	TYR	A	413	17.039	30.319	24.529	1.00	24.61
ATOM	879	CE1	TYR	A	413	16.122	29.840	25.472	1.00	21.19
ATOM	880	CD2	TYR	A	413	15.906	29.103	22.819	1.00	24.64
ATOM	881	CE2	TYR	A	413	14.991	28.629	23.739	1.00	26.94
ATOM	882	CZ	TYR	A	413	15.097	28.993	25.065	1.00	28.21
ATOM	883	OH	TYR	A	413	14.145	28.487	25.945	1.00	27.94
ATOM	884	C	TYR	A	413	19.906	29.164	22.453	1.00	23.48
ATOM	885	O	TYR	A	413	19.656	28.401	21.518	1.00	24.97
ATOM	886	N	PHE	A	414	20.684	28.828	23.488	1.00	22.58
ATOM	887	CA	PHE	A	414	21.360	27.534	23.625	1.00	21.94
ATOM	888	CB	PHE	A	414	22.835	27.685	23.195	1.00	18.84
ATOM	889	CG	PHE	A	414	23.734	26.507	23.555	1.00	23.28
ATOM	890	CD1	PHE	A	414	23.637	25.283	22.871	1.00	23.77
ATOM	891	CD2	PHE	A	414	24.718	26.634	24.556	1.00	20.51
ATOM	892	CE1	PHE	A	414	24.510	24.201	23.178	1.00	25.81
ATOM	893	CE2	PHE	A	414	25.586	25.569	24.865	1.00	17.09
ATOM	894	CZ	PHE	A	414	25.483	24.350	24.178	1.00	23.54
ATOM	895	C	PHE	A	414	21.303	26.977	25.057	1.00	25.66
ATOM	896	O	PHE	A	414	21.612	27.677	26.024	1.00	22.04
ATOM	897	N	ASP	A	415	20.866	25.731	25.196	1.00	25.08
ATOM	898	CA	ASP	A	415	20.849	25.114	26.513	1.00	22.21
ATOM	899	CB	ASP	A	415	22.303	24.853	26.921	1.00	17.07
ATOM	900	CG	ASP	A	415	22.441	23.735	27.894	1.00	18.13
ATOM	901	OD1	ASP	A	415	21.457	23.014	28.110	1.00	18.33
ATOM	902	OD2	ASP	A	415	23.551	23.579	28.420	1.00	20.42
ATOM	903	C	ASP	A	415	20.130	25.970	27.579	1.00	25.14
ATOM	904	O	ASP	A	415	20.700	26.259	28.633	1.00	29.15
ATOM	905	N	GLY	A	416	18.912	26.408	27.269	1.00	20.65
ATOM	906	CA	GLY	A	416	18.118	27.176	28.201	1.00	18.89
ATOM	907	C	GLY	A	416	18.258	28.682	28.257	1.00	13.58
ATOM	908	O	GLY	A	416	17.349	29.327	28.744	1.00	19.33
ATOM	909	N	LYS	A	417	19.364	29.254	27.817	1.00	14.55
ATOM	910	CA	LYS	A	417	19.498	30.716	27.861	1.00	18.31
ATOM	911	CB	LYS	A	417	20.345	31.134	29.074	1.00	20.71
ATOM	912	CG	LYS	A	417	19.682	30.877	30.428	1.00	22.06
ATOM	913	CD	LYS	A	417	20.679	31.167	31.538	1.00	23.89
ATOM	914	CE	LYS	A	417	19.970	31.232	32.891	1.00	26.28
ATOM	915	NZ	LYS	A	417	20.937	31.696	33.916	1.00	27.48
ATOM	916	C	LYS	A	417	20.183	31.202	26.592	1.00	23.82
ATOM	917	O	LYS	A	417	20.635	30.382	25.781	1.00	21.77
ATOM	918	N	TYR	A	418	20.315	32.526	26.443	1.00	21.57
ATOM	919	CA	TYR	A	418	20.972	33.115	25.270	1.00	19.31
ATOM	920	CB	TYR	A	418	20.369	34.492	24.921	1.00	18.21
ATOM	921	CG	TYR	A	418	19.066	34.407	24.142	1.00	21.12

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ATOM	922	CD1	TYR	A	418	17.856	34.087	24.777	1.00	18.03
ATOM	923	CE1	TYR	A	418	16.682	33.930	24.048	1.00	22.16
ATOM	924	CD2	TYR	A	418	19.060	34.576	22.743	1.00	19.41
ATOM	925	CE2	TYR	A	418	17.903	34.419	22.007	1.00	16.83
ATOM	926	CZ	TYR	A	418	16.728	34.099	22.648	1.00	24.12
ATOM	927	OH	TYR	A	418	15.601	33.944	21.890	1.00	22.47
ATOM	928	C	TYR	A	418	22.471	33.183	25.451	1.00	19.85
ATOM	929	O	TYR	A	418	22.974	33.820	26.385	1.00	25.51
ATOM	930	N	ALA	A	419	23.180	32.482	24.570	1.00	16.24
ATOM	931	CA	ALA	A	419	24.630	32.365	24.577	1.00	15.65
ATOM	932	CB	ALA	A	419	24.986	30.903	24.326	1.00	17.04
ATOM	933	C	ALA	A	419	25.463	33.245	23.629	1.00	25.93
ATOM	934	O	ALA	A	419	25.168	33.359	22.432	1.00	27.89
ATOM	935	N	SER	A	420	26.540	33.817	24.157	1.00	23.17
ATOM	936	CA	SER	A	420	27.455	34.619	23.360	1.00	24.99
ATOM	937	CB	SER	A	420	28.202	35.577	24.280	1.00	27.55
ATOM	938	OG	SER	A	420	29.050	34.861	25.170	1.00	31.44
ATOM	939	C	SER	A	420	28.442	33.622	22.735	1.00	25.61
ATOM	940	O	SER	A	420	28.462	32.461	23.132	1.00	26.24
ATOM	941	N	PRO	A	421	29.267	34.040	21.748	1.00	27.91
ATOM	942	CD	PRO	A	421	29.281	35.313	20.998	1.00	28.16
ATOM	943	CA	PRO	A	421	30.209	33.071	21.160	1.00	27.21
ATOM	944	CB	PRO	A	421	31.014	33.928	20.178	1.00	25.80
ATOM	945	CG	PRO	A	421	30.031	34.959	19.743	1.00	24.69
ATOM	946	C	PRO	A	421	31.158	32.380	22.163	1.00	34.03
ATOM	947	O	PRO	A	421	31.509	31.199	21.988	1.00	31.00
ATOM	948	N	ASP	A	422	31.627	33.142	23.158	1.00	33.32
ATOM	949	CA	ASP	A	422	32.570	32.623	24.154	1.00	35.81
ATOM	950	CB	ASP	A	422	33.136	33.742	25.030	1.00	44.04
ATOM	951	CG	ASP	A	422	32.246	34.946	25.069	1.00	54.68
ATOM	952	OD1	ASP	A	422	32.454	35.892	24.251	1.00	54.42
ATOM	953	OD2	ASP	A	422	31.327	34.920	25.913	1.00	58.40
ATOM	954	C	ASP	A	422	32.104	31.415	24.972	1.00	29.08
ATOM	955	O	ASP	A	422	32.923	30.698	25.550	1.00	29.48
ATOM	956	N	VAL	A	423	30.796	31.180	24.968	1.00	24.96
ATOM	957	CA	VAL	A	423	30.197	30.031	25.620	1.00	22.62
ATOM	958	CB	VAL	A	423	28.671	30.120	25.495	1.00	19.09
ATOM	959	CG1	VAL	A	423	28.025	28.771	25.617	1.00	20.56
ATOM	960	CG2	VAL	A	423	28.115	31.068	26.536	1.00	21.12
ATOM	961	C	VAL	A	423	30.724	28.783	24.894	1.00	26.71
ATOM	962	O	VAL	A	423	30.975	27.746	25.499	1.00	24.85
ATOM	963	N	PHE	A	424	31.040	28.951	23.611	1.00	26.18
ATOM	964	CA	PHE	A	424	31.507	27.854	22.774	1.00	22.48
ATOM	965	CB	PHE	A	424	30.860	27.963	21.371	1.00	23.86
ATOM	966	CG	PHE	A	424	29.341	28.011	21.394	1.00	20.24
ATOM	967	CD1	PHE	A	424	28.668	29.227	21.384	1.00	15.91
ATOM	968	CD2	PHE	A	424	28.598	26.843	21.509	1.00	15.76
ATOM	969	CE1	PHE	A	424	27.290	29.270	21.500	1.00	16.18
ATOM	970	CE2	PHE	A	424	27.238	26.880	21.623	1.00	13.58
ATOM	971	CZ	PHE	A	424	26.573	28.099	21.624	1.00	16.90
ATOM	972	C	PHE	A	424	33.014	27.757	22.663	1.00	23.66
ATOM	973	O	PHE	A	424	33.539	26.929	21.911	1.00	24.93
ATOM	974	N	LYS	A	425	33.727	28.552	23.451	1.00	26.33
ATOM	975	CA	LYS	A	425	35.186	28.527	23.392	1.00	29.12
ATOM	976	CB	LYS	A	425	35.776	29.467	24.452	1.00	32.35
ATOM	977	CG	LYS	A	425	37.306	29.529	24.457	1.00	31.98
ATOM	978	CD	LYS	A	425	37.762	30.593	25.418	1.00	39.70
ATOM	979	CE	LYS	A	425	39.265	30.718	25.450	1.00	48.00
ATOM	980	NZ	LYS	A	425	39.725	31.844	26.336	1.00	53.67
ATOM	981	C	LYS	A	425	35.889	27.157	23.476	1.00	31.57
ATOM	982	O	LYS	A	425	36.792	26.863	22.673	1.00	27.27
ATOM	983	N	SER	A	426	35.521	26.339	24.465	1.00	30.78
ATOM	984	CA	SER	A	426	36.182	25.050	24.607	1.00	33.82
ATOM	985	CB	SER	A	426	35.862	24.390	25.959	1.00	30.28
ATOM	986	OG	SER	A	426	34.486	24.161	26.133	1.00	37.92
ATOM	987	C	SER	A	426	35.992	24.104	23.417	1.00	35.48

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ATOM	988	O	SER A 426	36.713	23.122	23.286	1.00	37.65
ATOM	989	N	LEU A 427	35.109	24.463	22.488	1.00	35.14
ATOM	990	CA	LEU A 427	34.879	23.644	21.300	1.00	33.29
ATOM	991	CB	LEU A 427	33.771	24.270	20.461	1.00	30.08
ATOM	992	CG	LEU A 427	32.682	23.462	19.781	1.00	28.00
ATOM	993	CD1	LEU A 427	32.151	22.380	20.671	1.00	25.88
ATOM	994	CD2	LEU A 427	31.574	24.418	19.397	1.00	25.10
ATOM	995	C	LEU A 427	36.166	23.655	20.494	1.00	33.91
ATOM	996	O	LEU A 427	36.533	22.656	19.901	1.00	36.72
ATOM	997	N	GLY A 428	36.862	24.790	20.503	1.00	39.65
ATOM	998	CA	GLY A 428	38.105	24.932	19.750	1.00	40.93
ATOM	999	C	GLY A 428	37.884	25.241	18.269	1.00	43.39
ATOM	1000	O	GLY A 428	38.806	25.108	17.455	1.00	42.81
ATOM	1001	N	CYS A 429	36.670	25.685	17.927	1.00	43.35
ATOM	1002	CA	CYS A 429	36.291	25.995	16.544	1.00	43.84
ATOM	1003	CB	CYS A 429	35.025	25.224	16.176	1.00	43.95
ATOM	1004	SG	CYS A 429	35.244	23.452	16.181	1.00	50.28
ATOM	1005	C	CYS A 429	36.012	27.475	16.409	1.00	42.57
ATOM	1006	O	CYS A 429	35.003	27.873	15.838	1.00	39.45
ATOM	1007	N	GLU A 430	36.934	28.292	16.901	1.00	43.43
ATOM	1008	CA	GLU A 430	36.761	29.740	16.874	1.00	45.32
ATOM	1009	CB	GLU A 430	38.051	30.447	17.301	1.00	53.81
ATOM	1010	CG	GLU A 430	38.849	29.738	18.439	1.00	70.87
ATOM	1011	CD	GLU A 430	38.051	29.456	19.737	1.00	77.73
ATOM	1012	OE1	GLU A 430	37.138	30.245	20.098	1.00	80.51
ATOM	1013	OE2	GLU A 430	38.365	28.437	20.408	1.00	78.46
ATOM	1014	C	GLU A 430	36.236	30.320	15.552	1.00	40.15
ATOM	1015	O	GLU A 430	35.304	31.127	15.563	1.00	35.32
ATOM	1016	N	ASP A 431	36.782	29.870	14.420	1.00	36.97
ATOM	1017	CA	ASP A 431	36.355	30.383	13.101	1.00	37.50
ATOM	1018	CB	ASP A 431	37.352	30.007	12.009	1.00	45.12
ATOM	1019	CG	ASP A 431	38.743	30.507	12.303	1.00	50.38
ATOM	1020	OD1	ASP A 431	39.005	31.715	12.088	1.00	52.92
ATOM	1021	OD2	ASP A 431	39.564	29.686	12.767	1.00	58.71
ATOM	1022	C	ASP A 431	34.953	29.983	12.668	1.00	31.17
ATOM	1023	O	ASP A 431	34.169	30.832	12.249	1.00	29.39
ATOM	1024	N	PHE A 432	34.642	28.697	12.805	1.00	25.82
ATOM	1025	CA	PHE A 432	33.334	28.162	12.467	1.00	24.06
ATOM	1026	CB	PHE A 432	33.343	26.640	12.666	1.00	23.24
ATOM	1027	CG	PHE A 432	31.981	26.008	12.634	1.00	26.00
ATOM	1028	CD1	PHE A 432	31.359	25.728	11.428	1.00	24.09
ATOM	1029	CD2	PHE A 432	31.301	25.727	13.826	1.00	24.00
ATOM	1030	CE1	PHE A 432	30.077	25.182	11.407	1.00	25.60
ATOM	1031	CE2	PHE A 432	30.017	25.182	13.819	1.00	23.27
ATOM	1032	CZ	PHE A 432	29.399	24.907	12.608	1.00	27.15
ATOM	1033	C	PHE A 432	32.290	28.823	13.368	1.00	24.49
ATOM	1034	O	PHE A 432	31.166	29.081	12.939	1.00	23.40
ATOM	1035	N	ILE A 433	32.667	29.123	14.614	1.00	23.33
ATOM	1036	CA	ILE A 433	31.729	29.746	15.545	1.00	21.41
ATOM	1037	CB	ILE A 433	32.226	29.697	17.038	1.00	24.82
ATOM	1038	CG2	ILE A 433	31.307	30.551	17.946	1.00	24.79
ATOM	1039	CG1	ILE A 433	32.233	28.244	17.554	1.00	22.78
ATOM	1040	CD1	ILE A 433	30.846	27.630	17.696	1.00	21.04
ATOM	1041	C	ILE A 433	31.453	31.179	15.113	1.00	17.19
ATOM	1042	O	ILE A 433	30.293	31.589	15.046	1.00	21.19
ATOM	1043	N	SER A 434	32.491	31.937	14.770	1.00	23.08
ATOM	1044	CA	SER A 434	32.257	33.319	14.327	1.00	25.60
ATOM	1045	CB	SER A 434	33.561	34.097	14.162	1.00	28.06
ATOM	1046	OG	SER A 434	34.547	33.294	13.558	1.00	37.81
ATOM	1047	C	SER A 434	31.465	33.276	13.028	1.00	23.82
ATOM	1048	O	SER A 434	30.564	34.072	12.821	1.00	23.76
ATOM	1049	N	PHE A 435	31.752	32.279	12.199	1.00	24.82
ATOM	1050	CA	PHE A 435	31.034	32.096	10.947	1.00	24.08
ATOM	1051	CB	PHE A 435	31.646	30.923	10.161	1.00	26.80
ATOM	1052	CG	PHE A 435	31.106	30.767	8.748	1.00	30.19
ATOM	1053	CD1	PHE A 435	30.205	31.686	8.209	1.00	35.50

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ATOM	1054	CD2	PHE	A	435	31.487	29.678	7.961	1.00	33.97
ATOM	1055	CE1	PHE	A	435	29.684	31.523	6.906	1.00	34.39
ATOM	1056	CE2	PHE	A	435	30.977	29.505	6.657	1.00	34.83
ATOM	1057	CZ	PHE	A	435	30.074	30.430	6.136	1.00	31.71
ATOM	1058	C	PHE	A	435	29.548	31.844	11.264	1.00	26.45
ATOM	1059	O	PHE	A	435	28.665	32.480	10.688	1.00	28.86
ATOM	1060	N	VAL	A	436	29.255	30.967	12.223	1.00	22.48
ATOM	1061	CA	VAL	A	436	27.865	30.691	12.559	1.00	17.41
ATOM	1062	CB	VAL	A	436	27.757	29.624	13.695	1.00	17.64
ATOM	1063	CG1	VAL	A	436	26.377	29.570	14.228	1.00	22.49
ATOM	1064	CG2	VAL	A	436	28.122	28.278	13.195	1.00	17.15
ATOM	1065	C	VAL	A	436	27.164	31.978	12.991	1.00	17.44
ATOM	1066	O	VAL	A	436	26.053	32.278	12.534	1.00	18.61
ATOM	1067	N	PHE	A	437	27.803	32.741	13.874	1.00	19.96
ATOM	1068	CA	PHE	A	437	27.184	33.971	14.362	1.00	22.62
ATOM	1069	CB	PHE	A	437	27.946	34.539	15.573	1.00	24.58
ATOM	1070	CG	PHE	A	437	27.559	33.905	16.891	1.00	23.31
ATOM	1071	CD1	PHE	A	437	27.912	32.593	17.180	1.00	24.58
ATOM	1072	CD2	PHE	A	437	26.855	34.627	17.841	1.00	23.23
ATOM	1073	CE1	PHE	A	437	27.572	32.012	18.402	1.00	22.25
ATOM	1074	CE2	PHE	A	437	26.514	34.055	19.059	1.00	23.56
ATOM	1075	CZ	PHE	A	437	26.874	32.746	19.334	1.00	18.83
ATOM	1076	C	PHE	A	437	27.010	35.034	13.274	1.00	22.54
ATOM	1077	O	PHE	A	437	25.985	35.716	13.232	1.00	27.26
ATOM	1078	N	GLU	A	438	28.001	35.176	12.400	1.00	26.36
ATOM	1079	CA	GLU	A	438	27.898	36.157	11.302	1.00	27.43
ATOM	1080	CB	GLU	A	438	29.164	36.179	10.440	1.00	30.05
ATOM	1081	CG	GLU	A	438	29.073	37.131	9.227	1.00	31.17
ATOM	1082	CD	GLU	A	438	30.417	37.447	8.605	1.00	31.35
ATOM	1083	OE1	GLU	A	438	31.384	36.685	8.801	1.00	27.62
ATOM	1084	OE2	GLU	A	438	30.509	38.491	7.932	1.00	40.19
ATOM	1085	C	GLU	A	438	26.674	35.839	10.450	1.00	25.73
ATOM	1086	O	GLU	A	438	25.918	36.730	10.093	1.00	28.14
ATOM	1087	N	PHE	A	439	26.449	34.555	10.188	1.00	26.08
ATOM	1088	CA	PHE	A	439	25.292	34.118	9.433	1.00	24.60
ATOM	1089	CB	PHE	A	439	25.398	32.619	9.135	1.00	26.02
ATOM	1090	CG	PHE	A	439	24.280	32.098	8.283	1.00	27.70
ATOM	1091	CD1	PHE	A	439	24.304	32.270	6.904	1.00	29.06
ATOM	1092	CD2	PHE	A	439	23.177	31.483	8.855	1.00	31.10
ATOM	1093	CE1	PHE	A	439	23.251	31.842	6.123	1.00	24.89
ATOM	1094	CE2	PHE	A	439	22.111	31.050	8.069	1.00	31.13
ATOM	1095	CZ	PHE	A	439	22.153	31.234	6.701	1.00	28.01
ATOM	1096	C	PHE	A	439	23.964	34.426	10.162	1.00	28.45
ATOM	1097	O	PHE	A	439	22.958	34.770	9.518	1.00	28.20
ATOM	1098	N	GLY	A	440	23.926	34.257	11.491	1.00	26.29
ATOM	1099	CA	GLY	A	440	22.699	34.550	12.217	1.00	20.95
ATOM	1100	C	GLY	A	440	22.380	36.035	12.079	1.00	24.76
ATOM	1101	O	GLY	A	440	21.247	36.459	11.831	1.00	24.56
ATOM	1102	N	LYS	A	441	23.409	36.842	12.249	1.00	25.11
ATOM	1103	CA	LYS	A	441	23.283	38.290	12.135	1.00	31.81
ATOM	1104	CB	LYS	A	441	24.674	38.871	12.293	1.00	34.53
ATOM	1105	CG	LYS	A	441	24.720	40.343	12.482	1.00	48.07
ATOM	1106	CD	LYS	A	441	25.618	40.643	13.668	1.00	58.50
ATOM	1107	CE	LYS	A	441	25.088	39.955	14.934	1.00	61.35
ATOM	1108	NZ	LYS	A	441	25.698	40.550	16.152	1.00	67.81
ATOM	1109	C	LYS	A	441	22.741	38.659	10.733	1.00	34.70
ATOM	1110	O	LYS	A	441	21.767	39.411	10.579	1.00	32.85
ATOM	1111	N	SER	A	442	23.408	38.091	9.729	1.00	33.69
ATOM	1112	CA	SER	A	442	23.113	38.278	8.312	1.00	32.10
ATOM	1113	CB	SER	A	442	24.060	37.413	7.493	1.00	34.00
ATOM	1114	OG	SER	A	442	23.706	37.415	6.142	1.00	42.63
ATOM	1115	C	SER	A	442	21.699	37.939	7.953	1.00	29.45
ATOM	1116	O	SER	A	442	21.022	38.710	7.283	1.00	28.07
ATOM	1117	N	LEU	A	443	21.252	36.769	8.383	1.00	30.75
ATOM	1118	CA	LEU	A	443	19.903	36.341	8.091	1.00	28.97
ATOM	1119	CB	LEU	A	443	19.754	34.844	8.362	1.00	32.66



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ATOM	1120	CG	LEU	A	443	19.232	33.966	7.225	1.00	34.63
ATOM	1121	CD1	LEU	A	443	19.001	32.579	7.758	1.00	34.61
ATOM	1122	CD2	LEU	A	443	17.933	34.502	6.669	1.00	35.80
ATOM	1123	C	LEU	A	443	18.900	37.163	8.897	1.00	33.40
ATOM	1124	O	LEU	A	443	17.761	37.366	8.461	1.00	31.79
ATOM	1125	N	CYS	A	444	19.330	37.656	10.063	1.00	39.70
ATOM	1126	CA	CYS	A	444	18.474	38.478	10.937	1.00	44.50
ATOM	1127	CB	CYS	A	444	19.117	38.687	12.312	1.00	50.28
ATOM	1128	SG	CYS	A	444	18.752	37.411	13.539	1.00	54.66
ATOM	1129	C	CYS	A	444	18.177	39.845	10.346	1.00	44.03
ATOM	1130	O	CYS	A	444	17.053	40.343	10.468	1.00	42.14
ATOM	1131	N	SER	A	445	19.190	40.456	9.733	1.00	43.30
ATOM	1132	CA	SER	A	445	19.020	41.765	9.118	1.00	47.44
ATOM	1133	CB	SER	A	445	20.343	42.266	8.518	1.00	48.13
ATOM	1134	OG	SER	A	445	20.752	41.518	7.383	1.00	50.15
ATOM	1135	C	SER	A	445	17.885	41.815	8.071	1.00	48.45
ATOM	1136	O	SER	A	445	17.459	42.901	7.663	1.00	53.44
ATOM	1137	N	MET	A	446	17.393	40.656	7.636	1.00	44.69
ATOM	1138	CA	MET	A	446	16.306	40.631	6.665	1.00	43.05
ATOM	1139	CB	MET	A	446	16.389	39.386	5.789	1.00	40.50
ATOM	1140	CG	MET	A	446	17.577	39.419	4.842	1.00	41.60
ATOM	1141	SD	MET	A	446	17.833	37.906	3.917	1.00	47.28
ATOM	1142	CE	MET	A	446	19.506	37.667	4.191	1.00	42.50
ATOM	1143	C	MET	A	446	14.953	40.725	7.355	1.00	46.65
ATOM	1144	O	MET	A	446	13.971	41.150	6.746	1.00	50.18
ATOM	1145	N	HIS	A	447	14.921	40.382	8.643	1.00	46.34
ATOM	1146	CA	HIS	A	447	13.702	40.426	9.420	1.00	48.76
ATOM	1147	CB	HIS	A	447	13.259	41.882	9.589	1.00	60.69
ATOM	1148	CG	HIS	A	447	12.149	42.066	10.578	1.00	78.35
ATOM	1149	CD2	HIS	A	447	11.722	41.273	11.592	1.00	83.48
ATOM	1150	ND1	HIS	A	447	11.308	43.163	10.569	1.00	85.45
ATOM	1151	CE1	HIS	A	447	10.405	43.032	11.529	1.00	86.49
ATOM	1152	NE2	HIS	A	447	10.633	41.893	12.161	1.00	87.93
ATOM	1153	C	HIS	A	447	12.618	39.583	8.729	1.00	47.17
ATOM	1154	O	HIS	A	447	11.618	40.114	8.233	1.00	48.76
ATOM	1155	N	LEU	A	448	12.853	38.272	8.654	1.00	43.85
ATOM	1156	CA	LEU	A	448	11.922	37.320	8.021	1.00	37.21
ATOM	1157	CB	LEU	A	448	12.667	36.021	7.633	1.00	36.92
ATOM	1158	CG	LEU	A	448	14.004	36.045	6.867	1.00	36.45
ATOM	1159	CD1	LEU	A	448	14.486	34.629	6.601	1.00	35.34
ATOM	1160	CD2	LEU	A	448	13.867	36.798	5.553	1.00	41.17
ATOM	1161	C	LEU	A	448	10.703	36.961	8.887	1.00	34.64
ATOM	1162	O	LEU	A	448	10.847	36.731	10.083	1.00	35.66
ATOM	1163	N	THR	A	449	9.512	36.911	8.288	1.00	31.11
ATOM	1164	CA	THR	A	449	8.305	36.549	9.033	1.00	28.99
ATOM	1165	CB	THR	A	449	7.006	36.973	8.313	1.00	30.22
ATOM	1166	OG1	THR	A	449	6.777	36.098	7.201	1.00	29.38
ATOM	1167	CG2	THR	A	449	7.081	38.431	7.839	1.00	25.55
ATOM	1168	C	THR	A	449	8.271	35.030	9.134	1.00	29.64
ATOM	1169	O	THR	A	449	8.953	34.351	8.371	1.00	31.91
ATOM	1170	N	GLU	A	450	7.479	34.491	10.051	1.00	26.47
ATOM	1171	CA	GLU	A	450	7.392	33.047	10.182	1.00	27.53
ATOM	1172	CB	GLU	A	450	6.328	32.679	11.204	1.00	25.91
ATOM	1173	CG	GLU	A	450	6.730	33.026	12.617	1.00	27.73
ATOM	1174	CD	GLU	A	450	7.853	32.146	13.117	1.00	24.37
ATOM	1175	OE1	GLU	A	450	7.554	31.004	13.513	1.00	29.52
ATOM	1176	OE2	GLU	A	450	9.021	32.586	13.108	1.00	28.01
ATOM	1177	C	GLU	A	450	7.104	32.350	8.844	1.00	29.72
ATOM	1178	O	GLU	A	450	7.748	31.372	8.492	1.00	29.06
ATOM	1179	N	ASP	A	451	6.181	32.899	8.070	1.00	32.63
ATOM	1180	CA	ASP	A	451	5.830	32.306	6.780	1.00	30.31
ATOM	1181	CB	ASP	A	451	4.615	33.023	6.182	1.00	34.34
ATOM	1182	CG	ASP	A	451	3.314	32.660	6.891	1.00	39.42
ATOM	1183	OD1	ASP	A	451	3.330	31.766	7.755	1.00	42.60
ATOM	1184	OD2	ASP	A	451	2.261	33.254	6.573	1.00	46.92
ATOM	1185	C	ASP	A	451	7.005	32.321	5.813	1.00	27.29

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ATOM	1186	O	ASP	A	451	7.238	31.364	5.090	1.00	27.40
ATOM	1187	N	GLU	A	452	7.765	33.404	5.821	1.00	29.17
ATOM	1188	CA	GLU	A	452	8.928	33.510	4.946	1.00	33.64
ATOM	1189	CB	GLU	A	452	9.521	34.927	5.022	1.00	34.38
ATOM	1190	CG	GLU	A	452	8.592	35.990	4.410	1.00	38.12
ATOM	1191	CD	GLU	A	452	9.061	37.426	4.609	1.00	40.47
ATOM	1192	OE1	GLU	A	452	10.047	37.667	5.330	1.00	42.73
ATOM	1193	OE2	GLU	A	452	8.424	38.339	4.047	1.00	45.30
ATOM	1194	C	GLU	A	452	9.976	32.432	5.286	1.00	35.02
ATOM	1195	O	GLU	A	452	10.558	31.814	4.378	1.00	32.26
ATOM	1196	N	ILE	A	453	10.200	32.209	6.589	1.00	31.95
ATOM	1197	CA	ILE	A	453	11.159	31.194	7.061	1.00	28.64
ATOM	1198	CB	ILE	A	453	11.397	31.290	8.615	1.00	31.75
ATOM	1199	CG2	ILE	A	453	12.135	30.045	9.139	1.00	28.09
ATOM	1200	CG1	ILE	A	453	12.218	32.538	8.952	1.00	29.57
ATOM	1201	CD1	ILE	A	453	12.224	32.863	10.422	1.00	27.64
ATOM	1202	C	ILE	A	453	10.640	29.793	6.707	1.00	25.34
ATOM	1203	O	ILE	A	453	11.408	28.904	6.331	1.00	27.62
ATOM	1204	N	ALA	A	454	9.331	29.604	6.834	1.00	25.41
ATOM	1205	CA	ALA	A	454	8.698	28.317	6.524	1.00	28.05
ATOM	1206	CB	ALA	A	454	7.194	28.381	6.798	1.00	23.33
ATOM	1207	C	ALA	A	454	8.941	27.940	5.064	1.00	30.98
ATOM	1208	O	ALA	A	454	9.408	26.839	4.763	1.00	27.28
ATOM	1209	N	LEU	A	455	8.696	28.899	4.173	1.00	34.22
ATOM	1210	CA	LEU	A	455	8.850	28.677	2.744	1.00	33.15
ATOM	1211	CB	LEU	A	455	8.023	29.706	1.945	1.00	35.88
ATOM	1212	CG	LEU	A	455	6.504	29.399	1.973	1.00	35.93
ATOM	1213	CD1	LEU	A	455	5.706	30.626	1.672	1.00	39.84
ATOM	1214	CD2	LEU	A	455	6.159	28.277	0.989	1.00	32.00
ATOM	1215	C	LEU	A	455	10.307	28.601	2.328	1.00	30.16
ATOM	1216	O	LEU	A	455	10.676	27.724	1.540	1.00	32.09
ATOM	1217	N	PHE	A	456	11.150	29.460	2.894	1.00	26.03
ATOM	1218	CA	PHE	A	456	12.564	29.400	2.561	1.00	25.28
ATOM	1219	CB	PHE	A	456	13.313	30.595	3.142	1.00	27.10
ATOM	1220	CG	PHE	A	456	14.766	30.654	2.734	1.00	32.50
ATOM	1221	CD1	PHE	A	456	15.151	30.366	1.421	1.00	31.72
ATOM	1222	CD2	PHE	A	456	15.754	30.994	3.660	1.00	32.12
ATOM	1223	CE1	PHE	A	456	16.484	30.414	1.040	1.00	31.33
ATOM	1224	CE2	PHE	A	456	17.097	31.046	3.285	1.00	34.09
ATOM	1225	CZ	PHE	A	456	17.465	30.755	1.971	1.00	33.73
ATOM	1226	C	PHE	A	456	13.165	28.073	3.061	1.00	27.08
ATOM	1227	O	PHE	A	456	14.077	27.522	2.452	1.00	24.18
ATOM	1228	N	SER	A	457	12.626	27.547	4.162	1.00	26.66
ATOM	1229	CA	SER	A	457	13.084	26.278	4.719	1.00	24.70
ATOM	1230	CB	SER	A	457	12.366	25.986	6.034	1.00	22.68
ATOM	1231	OG	SER	A	457	12.761	26.899	7.025	1.00	28.15
ATOM	1232	C	SER	A	457	12.734	25.169	3.748	1.00	23.81
ATOM	1233	O	SER	A	457	13.561	24.315	3.425	1.00	21.55
ATOM	1234	N	ALA	A	458	11.470	25.154	3.337	1.00	24.49
ATOM	1235	CA	ALA	A	458	10.992	24.142	2.397	1.00	27.62
ATOM	1236	CB	ALA	A	458	9.526	24.345	2.126	1.00	26.08
ATOM	1237	C	ALA	A	458	11.811	24.190	1.095	1.00	25.57
ATOM	1238	O	ALA	A	458	12.205	23.161	0.571	1.00	28.96
ATOM	1239	N	PHE	A	459	12.153	25.399	0.660	1.00	27.37
ATOM	1240	CA	PHE	A	459	12.945	25.642	-0.553	1.00	28.58
ATOM	1241	CB	PHE	A	459	13.083	27.162	-0.758	1.00	28.53
ATOM	1242	CG	PHE	A	459	13.907	27.558	-1.956	1.00	33.04
ATOM	1243	CD1	PHE	A	459	13.402	27.404	-3.255	1.00	37.29
ATOM	1244	CD2	PHE	A	459	15.168	28.122	-1.789	1.00	32.57
ATOM	1245	CE1	PHE	A	459	14.142	27.809	-4.360	1.00	33.63
ATOM	1246	CE2	PHE	A	459	15.920	28.533	-2.886	1.00	36.16
ATOM	1247	CZ	PHE	A	459	15.407	28.378	-4.175	1.00	37.49
ATOM	1248	C	PHE	A	459	14.331	25.008	-0.495	1.00	28.01
ATOM	1249	O	PHE	A	459	14.743	24.252	-1.372	1.00	29.21
ATOM	1250	N	VAL	A	460	15.067	25.334	0.553	1.00	29.05
ATOM	1251	CA	VAL	A	460	16.407	24.798	0.701	1.00	26.40

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ATOM	1252	CB	VAL	A	460	17.143	25.531	1.839	1.00	28.85
ATOM	1253	CG1	VAL	A	460	18.470	24.967	2.044	1.00	34.54
ATOM	1254	CG2	VAL	A	460	17.319	26.974	1.484	1.00	30.19
ATOM	1255	C	VAL	A	460	16.385	23.268	0.889	1.00	24.40
ATOM	1256	O	VAL	A	460	17.295	22.563	0.447	1.00	25.65
ATOM	1257	N	LEU	A	461	15.307	22.743	1.469	1.00	24.80
ATOM	1258	CA	LEU	A	461	15.194	21.297	1.700	1.00	26.95
ATOM	1259	CB	LEU	A	461	14.034	21.015	2.653	1.00	28.61
ATOM	1260	CG	LEU	A	461	14.024	19.600	3.228	1.00	30.23
ATOM	1261	CD1	LEU	A	461	15.049	19.523	4.335	1.00	30.35
ATOM	1262	CD2	LEU	A	461	12.637	19.257	3.751	1.00	37.76
ATOM	1263	C	LEU	A	461	14.966	20.496	0.416	1.00	27.27
ATOM	1264	O	LEU	A	461	15.566	19.430	0.198	1.00	26.82
ATOM	1265	N	MET	A	462	14.023	20.991	-0.380	1.00	27.27
ATOM	1266	CA	MET	A	462	13.650	20.378	-1.640	1.00	30.35
ATOM	1267	CB	MET	A	462	12.196	20.707	-1.964	1.00	30.76
ATOM	1268	CG	MET	A	462	11.213	20.255	-0.874	1.00	41.65
ATOM	1269	SD	MET	A	462	11.153	18.462	-0.489	1.00	43.91
ATOM	1270	CE	MET	A	462	10.018	17.928	-1.767	1.00	47.33
ATOM	1271	C	MET	A	462	14.574	20.870	-2.730	1.00	29.93
ATOM	1272	O	MET	A	462	14.135	21.418	-3.729	1.00	33.71
ATOM	1273	N	SER	A	463	15.864	20.657	-2.524	1.00	30.81
ATOM	1274	CA	SER	A	463	16.881	21.064	-3.470	1.00	35.27
ATOM	1275	CB	SER	A	463	18.143	21.489	-2.730	1.00	36.89
ATOM	1276	OG	SER	A	463	18.963	22.273	-3.578	1.00	50.70
ATOM	1277	C	SER	A	463	17.174	19.889	-4.411	1.00	36.64
ATOM	1278	O	SER	A	463	17.599	18.819	-3.976	1.00	32.89
ATOM	1279	N	ALA	A	464	16.925	20.096	-5.702	1.00	39.89
ATOM	1280	CA	ALA	A	464	17.127	19.053	-6.698	1.00	40.73
ATOM	1281	CB	ALA	A	464	16.425	19.425	-7.980	1.00	39.42
ATOM	1282	C	ALA	A	464	18.585	18.728	-6.969	1.00	42.63
ATOM	1283	O	ALA	A	464	18.897	17.616	-7.401	1.00	48.91
ATOM	1284	N	ASP	A	465	19.481	19.663	-6.656	1.00	43.62
ATOM	1285	CA	ASP	A	465	20.905	19.461	-6.908	1.00	43.08
ATOM	1286	CB	ASP	A	465	21.546	20.754	-7.398	1.00	49.21
ATOM	1287	CG	ASP	A	465	21.620	21.805	-6.324	1.00	54.48
ATOM	1288	OD1	ASP	A	465	22.753	22.243	-6.029	1.00	56.04
ATOM	1289	OD2	ASP	A	465	20.555	22.184	-5.783	1.00	57.56
ATOM	1290	C	ASP	A	465	21.766	18.855	-5.803	1.00	41.94
ATOM	1291	O	ASP	A	465	22.946	19.191	-5.677	1.00	46.76
ATOM	1292	N	ARG	A	466	21.190	17.995	-4.976	1.00	37.97
ATOM	1293	CA	ARG	A	466	21.987	17.342	-3.953	1.00	34.33
ATOM	1294	CB	ARG	A	466	21.112	16.818	-2.804	1.00	31.22
ATOM	1295	CG	ARG	A	466	20.380	17.869	-2.006	1.00	27.68
ATOM	1296	CD	ARG	A	466	21.340	18.803	-1.302	1.00	27.64
ATOM	1297	NE	ARG	A	466	20.588	19.665	-0.400	1.00	26.47
ATOM	1298	CZ	ARG	A	466	21.076	20.728	0.234	1.00	24.01
ATOM	1299	NH1	ARG	A	466	22.341	21.082	0.092	1.00	20.35
ATOM	1300	NH2	ARG	A	466	20.266	21.477	0.969	1.00	25.10
ATOM	1301	C	ARG	A	466	22.613	16.155	-4.681	1.00	32.20
ATOM	1302	O	ARG	A	466	21.981	15.542	-5.543	1.00	34.80
ATOM	1303	N	SER	A	467	23.852	15.835	-4.343	1.00	31.72
ATOM	1304	CA	SER	A	467	24.512	14.700	-4.961	1.00	29.23
ATOM	1305	CB	SER	A	467	25.915	14.497	-4.373	1.00	30.36
ATOM	1306	OG	SER	A	467	26.750	15.613	-4.579	1.00	34.62
ATOM	1307	C	SER	A	467	23.705	13.442	-4.680	1.00	29.79
ATOM	1308	O	SER	A	467	23.050	13.327	-3.653	1.00	27.96
ATOM	1309	N	TRP	A	468	23.760	12.504	-5.610	1.00	27.51
ATOM	1310	CA	TRP	A	468	23.114	11.203	-5.476	1.00	27.13
ATOM	1311	CB	TRP	A	468	23.703	10.431	-4.286	1.00	30.38
ATOM	1312	CG	TRP	A	468	25.196	10.650	-4.109	1.00	33.34
ATOM	1313	CD2	TRP	A	468	26.241	10.375	-5.068	1.00	34.52
ATOM	1314	CE2	TRP	A	468	27.453	10.853	-4.510	1.00	34.97
ATOM	1315	CE3	TRP	A	468	26.271	9.778	-6.345	1.00	33.99
ATOM	1316	CD1	TRP	A	468	25.807	11.246	-3.043	1.00	35.05
ATOM	1317	NE1	TRP	A	468	27.152	11.376	-3.278	1.00	35.95

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ATOM	1318	CZ2	TRP	A	468	28.688	10.755	-5.182	1.00	32.97
ATOM	1319	CZ3	TRP	A	468	27.494	9.677	-7.012	1.00	29.70
ATOM	1320	CH2	TRP	A	468	28.686	10.167	-6.425	1.00	34.34
ATOM	1321	C	TRP	A	468	21.602	11.121	-5.472	1.00	27.07
ATOM	1322	O	TRP	A	468	21.042	10.084	-5.105	1.00	29.52
ATOM	1323	N	LEU	A	469	20.921	12.190	-5.874	1.00	27.42
ATOM	1324	CA	LEU	A	469	19.456	12.139	-5.945	1.00	30.07
ATOM	1325	CB	LEU	A	469	18.910	13.539	-6.099	1.00	28.28
ATOM	1326	CG	LEU	A	469	18.898	14.353	-4.824	1.00	24.65
ATOM	1327	CD1	LEU	A	469	18.463	15.758	-5.160	1.00	26.09
ATOM	1328	CD2	LEU	A	469	17.929	13.704	-3.867	1.00	20.08
ATOM	1329	C	LEU	A	469	19.028	11.294	-7.155	1.00	33.83
ATOM	1330	O	LEU	A	469	19.735	11.285	-8.146	1.00	39.39
ATOM	1331	N	GLN	A	470	17.916	10.564	-7.077	1.00	34.69
ATOM	1332	CA	GLN	A	470	17.463	9.757	-8.224	1.00	39.38
ATOM	1333	CB	GLN	A	470	16.832	8.443	-7.779	1.00	40.10
ATOM	1334	CG	GLN	A	470	17.796	7.485	-7.120	1.00	50.51
ATOM	1335	CD	GLN	A	470	17.111	6.245	-6.571	1.00	55.73
ATOM	1336	OE1	GLN	A	470	15.993	5.911	-6.964	1.00	57.73
ATOM	1337	NE2	GLN	A	470	17.776	5.565	-5.643	1.00	58.82
ATOM	1338	C	GLN	A	470	16.444	10.524	-9.050	1.00	40.91
ATOM	1339	O	GLN	A	470	16.619	10.727	-10.250	1.00	42.98
ATOM	1340	N	GLU	A	471	15.383	10.960	-8.386	1.00	40.83
ATOM	1341	CA	GLU	A	471	14.308	11.720	-9.013	1.00	40.88
ATOM	1342	CB	GLU	A	471	13.001	11.447	-8.269	1.00	40.93
ATOM	1343	CG	GLU	A	471	12.699	9.972	-8.077	1.00	48.61
ATOM	1344	CD	GLU	A	471	11.560	9.737	-7.098	1.00	53.74
ATOM	1345	OE1	GLU	A	471	10.392	10.051	-7.438	1.00	52.66
ATOM	1346	OE2	GLU	A	471	11.841	9.243	-5.981	1.00	59.20
ATOM	1347	C	GLU	A	471	14.588	13.235	-9.046	1.00	41.53
ATOM	1348	O	GLU	A	471	13.780	14.027	-8.551	1.00	42.72
ATOM	1349	N	LYS	A	472	15.707	13.634	-9.657	1.00	41.50
ATOM	1350	CA	LYS	A	472	16.086	15.044	-9.750	1.00	41.09
ATOM	1351	CB	LYS	A	472	17.332	15.198	-10.614	1.00	38.72
ATOM	1352	CG	LYS	A	472	19.592	14.669	-9.971	1.00	43.30
ATOM	1353	CD	LYS	A	472	19.731	15.695	-10.033	1.00	46.29
ATOM	1354	CE	LYS	A	472	20.679	15.517	-8.831	1.00	50.44
ATOM	1355	NZ	LYS	A	472	21.892	16.398	-8.804	1.00	46.13
ATOM	1356	C	LYS	A	472	14.978	15.941	-10.287	1.00	43.56
ATOM	1357	O	LYS	A	472	14.628	16.963	-9.689	1.00	43.75
ATOM	1358	N	VAL	A	473	14.399	15.511	-11.402	1.00	46.51
ATOM	1359	CA	VAL	A	473	13.326	16.236	-12.084	1.00	43.88
ATOM	1360	CB	VAL	A	473	12.963	15.516	-13.416	1.00	49.53
ATOM	1361	CG1	VAL	A	473	11.696	16.128	-14.040	1.00	51.00
ATOM	1362	CG2	VAL	A	473	14.155	15.611	-14.395	1.00	49.56
ATOM	1363	C	VAL	A	473	12.076	16.466	-11.235	1.00	37.01
ATOM	1364	O	VAL	A	473	11.536	17.572	-11.212	1.00	33.80
ATOM	1365	N	LYS	A	474	11.609	15.415	-10.570	1.00	36.39
ATOM	1366	CA	LYS	A	474	10.440	15.508	-9.695	1.00	36.93
ATOM	1367	CB	LYS	A	474	10.084	14.126	-9.147	1.00	35.35
ATOM	1368	CG	LYS	A	474	8.886	14.077	-8.218	1.00	38.41
ATOM	1369	CD	LYS	A	474	8.579	12.626	-7.848	1.00	46.48
ATOM	1370	CE	LYS	A	474	7.746	12.480	-6.569	1.00	53.40
ATOM	1371	NZ	LYS	A	474	6.298	12.790	-6.709	1.00	57.86
ATOM	1372	C	LYS	A	474	10.713	16.495	-8.537	1.00	37.36
ATOM	1373	O	LYS	A	474	9.887	17.359	-8.250	1.00	36.85
ATOM	1374	N	ILE	A	475	11.897	16.422	-7.927	1.00	37.31
ATOM	1375	CA	ILE	A	475	12.231	17.328	-6.820	1.00	37.61
ATOM	1376	CB	ILE	A	475	13.535	16.887	-6.067	1.00	35.04
ATOM	1377	CG2	ILE	A	475	13.834	17.877	-4.931	1.00	34.59
ATOM	1378	CG1	ILE	A	475	13.368	15.464	-5.488	1.00	27.42
ATOM	1379	CD1	ILE	A	475	14.680	14.711	-5.243	1.00	18.44
ATOM	1380	C	ILE	A	475	12.349	18.766	-7.352	1.00	40.05
ATOM	1381	O	ILE	A	475	11.882	19.727	-6.721	1.00	38.84
ATOM	1382	N	GLU	A	476	12.913	18.896	-8.550	1.00	41.69
ATOM	1383	CA	GLU	A	476	13.066	20.184	-9.207	1.00	43.30

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ATOM	1384	CB	GLU	A	476	13.755	19.984	-10.552	1.00	48.95
ATOM	1385	CG	GLU	A	476	13.732	21.196	-11.464	1.00	62.73
ATOM	1386	CD	GLU	A	476	14.355	22.442	-10.846	1.00	70.08
ATOM	1387	OE1	GLU	A	476	15.464	22.338	-10.274	1.00	76.26
ATOM	1388	OE2	GLU	A	476	13.741	23.532	-10.947	1.00	75.60
ATOM	1389	C	GLU	A	476	11.705	20.850	-9.413	1.00	42.70
ATOM	1390	O	GLU	A	476	11.547	22.050	-9.183	1.00	38.37
ATOM	1391	N	LYS	A	477	10.724	20.066	-9.854	1.00	41.95
ATOM	1392	CA	LYS	A	477	9.379	20.580	-10.072	1.00	45.24
ATOM	1393	CB	LYS	A	477	8.461	19.496	-10.643	1.00	49.85
ATOM	1394	CG	LYS	A	477	8.971	18.848	-11.905	1.00	59.55
ATOM	1395	CD	LYS	A	477	9.158	19.879	-12.984	1.00	69.14
ATOM	1396	CE	LYS	A	477	9.721	19.258	-14.243	1.00	75.50
ATOM	1397	NZ	LYS	A	477	9.631	20.220	-15.382	1.00	82.60
ATOM	1398	C	LYS	A	477	8.798	21.075	-8.753	1.00	45.20
ATOM	1399	O	LYS	A	477	8.303	22.207	-8.668	1.00	44.88
ATOM	1400	N	LEU	A	478	8.850	20.216	-7.728	1.00	42.02
ATOM	1401	CA	LEU	A	478	8.339	20.575	-6.403	1.00	39.03
ATOM	1402	CB	LEU	A	478	8.506	19.411	-5.419	1.00	38.50
ATOM	1403	CG	LEU	A	478	7.562	18.213	-5.609	1.00	38.77
ATOM	1404	CD1	LEU	A	478	7.919	17.062	-4.658	1.00	40.42
ATOM	1405	CD2	LEU	A	478	6.126	18.653	-5.389	1.00	36.80
ATOM	1406	C	LEU	A	478	9.020	21.856	-5.875	1.00	37.92
ATOM	1407	O	LEU	A	478	8.332	22.767	-5.399	1.00	37.49
ATOM	1408	N	GLN	A	479	10.344	21.963	-6.057	1.00	37.80
ATOM	1409	CA	GLN	A	479	11.083	23.144	-5.607	1.00	38.11
ATOM	1410	CB	GLN	A	479	12.610	22.987	-5.772	1.00	36.91
ATOM	1411	CG	GLN	A	479	13.425	24.177	-5.189	1.00	40.17
ATOM	1412	CD	GLN	A	479	14.938	24.122	-5.452	1.00	42.02
ATOM	1413	OE1	GLN	A	479	15.411	23.469	-6.392	1.00	48.01
ATOM	1414	NE2	GLN	A	479	15.702	24.820	-4.616	1.00	46.19
ATOM	1415	C	GLN	A	479	10.589	24.379	-6.343	1.00	39.25
ATOM	1416	O	GLN	A	479	10.392	25.426	-5.718	1.00	42.08
ATOM	1417	N	GLN	A	480	10.348	24.251	-7.650	1.00	39.34
ATOM	1418	CA	GLN	A	480	9.955	25.371	-8.460	1.00	43.07
ATOM	1419	CB	GLN	A	480	9.547	24.917	-9.894	1.00	51.07
ATOM	1420	CG	GLN	A	480	10.733	24.407	-10.707	1.00	64.44
ATOM	1421	CD	GLN	A	480	10.291	23.533	-11.889	1.00	73.00
ATOM	1422	OE1	GLN	A	480	9.132	23.582	-12.310	1.00	75.34
ATOM	1423	NE2	GLN	A	480	11.211	22.732	-12.425	1.00	72.93
ATOM	1424	C	GLN	A	480	8.591	25.987	-7.853	1.00	37.24
ATOM	1425	O	GLN	A	480	8.499	27.198	-7.658	1.00	35.48
ATOM	1426	N	LYS	A	481	7.620	25.139	-7.545	1.00	35.17
ATOM	1427	CA	LYS	A	481	6.381	25.614	-6.957	1.00	37.36
ATOM	1428	CB	LYS	A	481	5.397	24.470	-6.801	1.00	41.26
ATOM	1429	CG	LYS	A	481	4.877	23.975	-8.112	1.00	49.18
ATOM	1430	CD	LYS	A	481	3.683	23.105	-7.907	1.00	59.24
ATOM	1431	CE	LYS	A	481	2.989	22.839	-9.229	1.00	68.40
ATOM	1432	NZ	LYS	A	481	1.798	21.950	-9.050	1.00	76.15
ATOM	1433	C	LYS	A	481	6.599	26.317	-5.628	1.00	37.73
ATOM	1434	O	LYS	A	481	5.976	27.353	-5.360	1.00	35.72
ATOM	1435	N	ILE	A	482	7.486	25.748	-4.806	1.00	38.76
ATOM	1436	CA	ILE	A	482	7.831	26.299	-3.494	1.00	36.16
ATOM	1437	CB	ILE	A	482	8.817	25.381	-2.705	1.00	32.89
ATOM	1438	CG2	ILE	A	482	9.404	26.130	-1.514	1.00	34.55
ATOM	1439	CG1	ILE	A	482	8.112	24.093	-2.234	1.00	28.40
ATOM	1440	CD1	ILE	A	482	9.070	23.005	-1.769	1.00	24.86
ATOM	1441	C	ILE	A	482	8.447	27.681	-3.639	1.00	35.37
ATOM	1442	O	ILE	A	482	8.152	28.579	-2.864	1.00	36.18
ATOM	1443	N	GLN	A	483	9.256	27.862	-4.668	1.00	38.47
ATOM	1444	CA	GLN	A	483	9.867	29.164	-4.892	1.00	39.76
ATOM	1445	CB	GLN	A	483	10.932	29.071	-5.950	1.00	40.59
ATOM	1446	CG	GLN	A	483	11.712	30.342	-6.053	1.00	49.20
ATOM	1447	CD	GLN	A	483	12.711	30.296	-7.192	1.00	58.50
ATOM	1448	OE1	GLN	A	483	12.820	29.303	-7.861	1.00	65.68
ATOM	1449	NE2	GLN	A	483	13.440	31.368	-7.409	1.00	65.23

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ATOM	1450	C	GLN	A	483	8.843	30.239	-5.284	1.00	40.84
ATOM	1451	O	GLN	A	483	8.969	31.422	-4.923	1.00	38.66
ATOM	1452	N	LEU	A	484	7.802	29.820	-6.002	1.00	39.88
ATOM	1453	CA	LEU	A	484	6.754	30.730	-6.439	1.00	42.14
ATOM	1454	CB	LEU	A	484	5.812	30.033	-7.416	1.00	45.74
ATOM	1455	CG	LEU	A	484	6.403	29.624	-8.765	1.00	48.71
ATOM	1456	CD1	LEU	A	484	5.337	28.943	-9.615	1.00	48.20
ATOM	1457	CD2	LEU	A	484	6.966	30.856	-9.472	1.00	50.22
ATOM	1458	C	LEU	A	484	5.957	31.241	-5.252	1.00	42.55
ATOM	1459	O	LEU	A	484	5.622	32.424	-5.181	1.00	42.64
ATOM	1460	N	ALA	A	485	5.626	30.329	-4.338	1.00	43.56
ATOM	1461	CA	ALA	A	485	4.872	30.672	-3.128	1.00	40.84
ATOM	1462	CB	ALA	A	485	4.350	29.403	-2.449	1.00	41.40
ATOM	1463	C	ALA	A	485	5.729	31.497	-2.162	1.00	37.33
ATOM	1464	O	ALA	A	485	5.204	32.298	-1.388	1.00	37.52
ATOM	1465	N	LEU	A	486	7.047	31.293	-2.215	1.00	35.33
ATOM	1466	CA	LEU	A	486	7.979	32.036	-1.380	1.00	38.02
ATOM	1467	CB	LEU	A	486	9.371	31.401	-1.395	1.00	32.53
ATOM	1468	CG	LEU	A	486	10.451	32.287	-0.758	1.00	33.21
ATOM	1469	CD1	LEU	A	486	10.176	32.478	0.723	1.00	32.27
ATOM	1470	CD2	LEU	A	486	11.818	31.693	-0.965	1.00	31.01
ATOM	1471	C	LEU	A	486	8.049	33.457	-1.942	1.00	42.86
ATOM	1472	O	LEU	A	486	8.077	34.446	-1.190	1.00	44.35
ATOM	1473	N	GLN	A	487	8.070	33.545	-3.271	1.00	44.64
ATOM	1474	CA	GLN	A	487	8.112	34.813	-3.998	1.00	47.16
ATOM	1475	CB	GLN	A	487	8.145	34.502	-5.486	1.00	51.86
ATOM	1476	CG	GLN	A	487	9.000	35.408	-6.310	1.00	61.53
ATOM	1477	CD	GLN	A	487	9.486	34.714	-7.571	1.00	65.93
ATOM	1478	OE1	GLN	A	487	9.083	33.587	-7.865	1.00	66.76
ATOM	1479	NE2	GLN	A	487	10.369	35.373	-8.311	1.00	70.60
ATOM	1480	C	GLN	A	487	6.823	35.579	-3.655	1.00	47.05
ATOM	1481	O	GLN	A	487	6.844	36.754	-3.307	1.00	45.17
ATOM	1482	N	HIS	A	488	5.702	34.874	-3.741	1.00	47.07
ATOM	1483	CA	HIS	A	488	4.387	35.405	-3.423	1.00	48.67
ATOM	1484	CB	HIS	A	488	3.374	34.280	-3.608	1.00	51.60
ATOM	1485	CG	HIS	A	488	2.095	34.484	-2.868	1.00	59.15
ATOM	1486	CD2	HIS	A	488	1.638	33.939	-1.715	1.00	62.57
ATOM	1487	ND1	HIS	A	488	1.097	35.317	-3.322	1.00	63.45
ATOM	1488	CE1	HIS	A	488	0.074	35.272	-2.485	1.00	64.94
ATOM	1489	NE2	HIS	A	488	0.378	34.444	-1.500	1.00	65.61
ATOM	1490	C	HIS	A	488	4.334	35.962	-1.986	1.00	49.05
ATOM	1491	O	HIS	A	488	3.925	37.097	-1.757	1.00	48.47
ATOM	1492	N	VAL	A	489	4.755	35.154	-1.021	1.00	48.07
ATOM	1493	CA	VAL	A	489	4.763	35.571	0.381	1.00	45.44
ATOM	1494	CB	VAL	A	489	5.220	34.401	1.302	1.00	46.07
ATOM	1495	CG1	VAL	A	489	5.592	34.911	2.692	1.00	44.85
ATOM	1496	CG2	VAL	A	489	4.115	33.372	1.409	1.00	41.76
ATOM	1497	C	VAL	A	489	5.682	36.773	0.580	1.00	43.28
ATOM	1498	O	VAL	A	489	5.319	37.741	1.229	1.00	41.87
ATOM	1499	N	LEU	A	490	6.866	36.706	-0.006	1.00	44.44
ATOM	1500	CA	LEU	A	490	7.865	37.763	0.103	1.00	49.79
ATOM	1501	CB	LEU	A	490	9.075	37.410	-0.766	1.00	50.68
ATOM	1502	CG	LEU	A	490	10.389	36.884	-0.181	1.00	54.00
ATOM	1503	CD1	LEU	A	490	10.223	36.100	1.115	1.00	54.10
ATOM	1504	CD2	LEU	A	490	11.034	36.035	-1.241	1.00	54.17
ATOM	1505	C	LEU	A	490	7.338	39.122	-0.310	1.00	52.92
ATOM	1506	O	LEU	A	490	7.224	40.037	0.498	1.00	50.59
ATOM	1507	N	GLN	A	491	7.014	39.243	-1.587	1.00	60.06
ATOM	1508	CA	GLN	A	491	6.513	40.494	-2.107	1.00	66.69
ATOM	1509	CB	GLN	A	491	6.560	40.523	-3.638	1.00	72.00
ATOM	1510	CG	GLN	A	491	6.078	39.292	-4.373	1.00	75.89
ATOM	1511	CD	GLN	A	491	6.340	39.394	-5.862	1.00	79.38
ATOM	1512	OE1	GLN	A	491	7.133	40.231	-6.302	1.00	82.32
ATOM	1513	NE2	GLN	A	491	5.672	38.554	-6.647	1.00	81.82
ATOM	1514	C	GLN	A	491	5.144	40.863	-1.555	1.00	68.27
ATOM	1515	O	GLN	A	491	4.820	42.045	-1.433	1.00	69.36

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ATOM	1516	N	LYS	A	492	4.360	39.863	-1.168	1.00	69.33
ATOM	1517	CA	LYS	A	492	3.055	40.123	-0.581	1.00	70.57
ATOM	1518	CB	LYS	A	492	2.464	38.825	-0.036	1.00	63.87
ATOM	1519	CG	LYS	A	492	1.419	39.011	1.021	1.00	55.18
ATOM	1520	CD	LYS	A	492	0.936	37.684	1.518	1.00	50.15
ATOM	1521	CE	LYS	A	492	0.170	36.960	0.445	1.00	47.92
ATOM	1522	NZ	LYS	A	492	-0.429	35.700	0.955	1.00	49.79
ATOM	1523	C	LYS	A	492	3.258	41.101	0.561	1.00	76.10
ATOM	1524	O	LYS	A	492	2.447	41.991	0.778	1.00	78.57
ATOM	1525	N	ASN	A	493	4.387	40.955	1.245	1.00	83.09
ATOM	1526	CA	ASN	A	493	4.724	41.795	2.380	1.00	90.65
ATOM	1527	CB	ASN	A	493	5.326	40.936	3.510	1.00	91.76
ATOM	1528	CG	ASN	A	493	4.413	39.791	3.960	1.00	91.33
ATOM	1529	OD1	ASN	A	493	3.483	39.989	4.743	1.00	90.45
ATOM	1530	ND2	ASN	A	493	4.727	38.576	3.525	1.00	90.60
ATOM	1531	C	ASN	A	493	5.703	42.929	2.053	1.00	96.54
ATOM	1532	O	ASN	A	493	5.445	44.097	2.361	1.00	97.40
ATOM	1533	N	HIS	A	494	6.815	42.593	1.401	1.00	104.63
ATOM	1534	CA	HIS	A	494	7.847	43.592	1.111	1.00	112.99
ATOM	1535	CB	HIS	A	494	9.092	43.302	1.972	1.00	118.20
ATOM	1536	CG	HIS	A	494	8.776	42.865	3.375	1.00	123.22
ATOM	1537	CD2	HIS	A	494	8.606	41.630	3.906	1.00	124.65
ATOM	1538	ND1	HIS	A	494	8.580	43.754	4.409	1.00	125.31
ATOM	1539	CE1	HIS	A	494	8.306	43.087	5.517	1.00	125.71
ATOM	1540	NE2	HIS	A	494	8.314	41.796	5.238	1.00	124.45
ATOM	1541	C	HIS	A	494	8.283	43.810	-0.343	1.00	115.21
ATOM	1542	O	HIS	A	494	9.414	43.476	-0.719	1.00	113.88
ATOM	1543	N	ARG	A	495	7.411	44.411	-1.150	1.00	118.74
ATOM	1544	CA	ARG	A	495	7.771	44.693	-2.539	1.00	123.08
ATOM	1545	CB	ARG	A	495	6.532	44.895	-3.411	1.00	124.19
ATOM	1546	CG	ARG	A	495	5.922	43.611	-3.923	1.00	125.95
ATOM	1547	CD	ARG	A	495	4.905	43.869	-5.022	1.00	128.86
ATOM	1548	NE	ARG	A	495	4.097	42.688	-5.336	1.00	130.65
ATOM	1549	CZ	ARG	A	495	2.771	42.700	-5.469	1.00	131.44
ATOM	1550	NH1	ARG	A	495	2.089	43.929	-5.316	1.00	132.26
ATOM	1551	NH2	ARG	A	495	2.122	41.580	-5.755	1.00	132.05
ATOM	1552	C	ARG	A	495	8.677	45.927	-2.632	1.00	124.82
ATOM	1553	O	ARG	A	495	9.086	46.332	-3.723	1.00	125.80
ATOM	1554	N	GLU	A	496	8.979	46.520	-1.479	1.00	125.27
ATOM	1555	CA	GLU	A	496	9.840	47.694	-1.403	1.00	125.62
ATOM	1556	CB	GLU	A	496	10.086	48.053	0.060	1.00	125.24
ATOM	1557	CG	GLU	A	496	10.364	46.856	0.953	1.00	125.43
ATOM	1558	CD	GLU	A	496	10.161	47.175	2.414	1.00	127.70
ATOM	1559	OE1	GLU	A	496	11.014	47.880	2.992	1.00	129.15
ATOM	1560	OE2	GLU	A	496	9.137	46.733	2.981	1.00	127.94
ATOM	1561	C	GLU	A	496	11.162	47.439	-2.117	1.00	126.43
ATOM	1562	O	GLU	A	496	11.731	48.346	-2.723	1.00	127.96
ATOM	1563	N	ASP	A	497	11.635	46.195	-2.047	1.00	126.16
ATOM	1564	CA	ASP	A	497	12.886	45.790	-2.693	1.00	124.22
ATOM	1565	CB	ASP	A	497	14.036	45.643	-1.669	1.00	124.95
ATOM	1566	CG	ASP	A	497	13.719	46.260	-0.317	1.00	125.55
ATOM	1567	OD1	ASP	A	497	13.970	47.468	-0.132	1.00	125.55
ATOM	1568	OD2	ASP	A	497	13.221	45.530	0.565	1.00	126.80
ATOM	1569	C	ASP	A	497	12.646	44.446	-3.392	1.00	121.48
ATOM	1570	O	ASP	A	497	11.524	44.142	-3.807	1.00	121.28
ATOM	1571	N	GLY	A	498	13.711	43.655	-3.527	1.00	118.36
ATOM	1572	CA	GLY	A	498	13.637	42.337	-4.142	1.00	112.17
ATOM	1573	C	GLY	A	498	14.617	41.465	-3.374	1.00	106.96
ATOM	1574	O	GLY	A	498	15.677	41.104	-3.889	1.00	107.39
ATOM	1575	N	ILE	A	499	14.253	41.158	-2.128	1.00	100.38
ATOM	1576	CA	ILE	A	499	15.058	40.378	-1.187	1.00	90.88
ATOM	1577	CB	ILE	A	499	14.545	40.644	0.259	1.00	89.37
ATOM	1578	CG2	ILE	A	499	14.172	39.362	0.988	1.00	88.94
ATOM	1579	CG1	ILE	A	499	15.573	41.483	1.013	1.00	88.59
ATOM	1580	CD1	ILE	A	499	16.015	42.736	0.254	1.00	88.83
ATOM	1581	C	ILE	A	499	15.254	38.885	-1.469	1.00	85.97

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ATOM	1582	O	ILE	A	499	16.120	38.243	-0.872	1.00	81.39
ATOM	1583	N	LEU	A	500	14.482	38.353	-2.412	1.00	82.32
ATOM	1584	CA	LEU	A	500	14.572	36.945	-2.784	1.00	79.33
ATOM	1585	CB	LEU	A	500	13.593	36.610	-3.926	1.00	75.45
ATOM	1586	CG	LEU	A	500	13.480	35.160	-4.427	1.00	72.35
ATOM	1587	CD1	LEU	A	500	13.020	34.209	-3.345	1.00	70.46
ATOM	1588	CD2	LEU	A	500	12.509	35.104	-5.569	1.00	74.01
ATOM	1589	C	LEU	A	500	15.994	36.594	-3.191	1.00	78.86
ATOM	1590	O	LEU	A	500	16.443	35.483	-2.943	1.00	80.08
ATOM	1591	N	THR	A	501	16.709	37.548	-3.786	1.00	78.15
ATOM	1592	CA	THR	A	501	18.085	37.316	-4.224	1.00	79.02
ATOM	1593	CB	THR	A	501	18.654	38.487	-5.065	1.00	82.06
ATOM	1594	OG1	THR	A	501	18.870	39.635	-4.225	1.00	84.30
ATOM	1595	CG2	THR	A	501	17.708	38.834	-6.214	1.00	83.64
ATOM	1596	C	THR	A	501	18.935	37.193	-2.988	1.00	77.23
ATOM	1597	O	THR	A	501	19.694	36.236	-2.831	1.00	77.82
ATOM	1598	N	LYS	A	502	18.776	38.185	-2.117	1.00	74.83
ATOM	1599	CA	LYS	A	502	19.478	38.276	-0.847	1.00	72.92
ATOM	1600	CB	LYS	A	502	18.834	39.402	-0.025	1.00	79.85
ATOM	1601	CG	LYS	A	502	19.726	40.108	0.995	1.00	85.84
ATOM	1602	CD	LYS	A	502	18.937	41.231	1.690	1.00	89.85
ATOM	1603	CE	LYS	A	502	19.744	41.963	2.764	1.00	94.60
ATOM	1604	NZ	LYS	A	502	18.918	42.984	3.487	1.00	95.90
ATOM	1605	C	LYS	A	502	19.282	36.922	-0.158	1.00	66.91
ATOM	1606	O	LYS	A	502	20.227	36.332	0.360	1.00	65.72
ATOM	1607	N	LEU	A	503	18.060	36.409	-0.267	1.00	59.20
ATOM	1608	CA	LEU	A	503	17.662	35.134	0.306	1.00	52.88
ATOM	1609	CB	LEU	A	503	16.158	34.971	0.156	1.00	47.50
ATOM	1610	CG	LEU	A	503	15.466	34.377	1.365	1.00	49.58
ATOM	1611	CD1	LEU	A	503	16.066	34.928	2.664	1.00	46.78
ATOM	1612	CD2	LEU	A	503	13.990	34.688	1.270	1.00	51.22
ATOM	1613	C	LEU	A	503	18.374	33.938	-0.314	1.00	51.55
ATOM	1614	O	LEU	A	503	19.200	33.301	0.334	1.00	49.38
ATOM	1615	N	ILE	A	504	18.087	33.645	-1.579	1.00	50.92
ATOM	1616	CA	ILE	A	504	18.715	32.499	-2.231	1.00	51.60
ATOM	1617	CB	ILE	A	504	18.054	32.153	-3.588	1.00	55.42
ATOM	1618	CG2	ILE	A	504	16.718	31.464	-3.360	1.00	52.28
ATOM	1619	CG1	ILE	A	504	17.860	33.415	-4.418	1.00	59.46
ATOM	1620	CD1	ILE	A	504	16.623	33.368	-5.320	1.00	67.68
ATOM	1621	C	ILE	A	504	20.233	32.598	-2.336	1.00	49.75
ATOM	1622	O	ILE	A	504	20.917	31.593	-2.485	1.00	50.38
ATOM	1623	N	CYS	A	505	20.773	33.798	-2.192	1.00	48.02
ATOM	1624	CA	CYS	A	505	22.221	33.974	-2.220	1.00	49.31
ATOM	1625	CB	CYS	A	505	22.557	35.465	-2.457	1.00	58.96
ATOM	1626	SG	CYS	A	505	23.762	36.304	-1.354	1.00	77.11
ATOM	1627	C	CYS	A	505	22.791	33.433	-0.891	1.00	46.24
ATOM	1628	O	CYS	A	505	23.956	33.014	-0.803	1.00	41.30
ATOM	1629	N	LYS	A	506	21.939	33.398	0.131	1.00	40.06
ATOM	1630	CA	LYS	A	506	22.336	32.890	1.425	1.00	37.35
ATOM	1631	CB	LYS	A	506	21.286	33.221	2.481	1.00	40.11
ATOM	1632	CG	LYS	A	506	20.957	34.686	2.596	1.00	43.49
ATOM	1633	CD	LYS	A	506	22.217	35.514	2.611	1.00	51.34
ATOM	1634	CE	LYS	A	506	22.343	36.269	3.891	1.00	55.65
ATOM	1635	NZ	LYS	A	506	22.139	35.376	5.071	1.00	63.77
ATOM	1636	C	LYS	A	506	22.466	31.389	1.309	1.00	36.27
ATOM	1637	O	LYS	A	506	23.267	30.786	2.005	1.00	40.04
ATOM	1638	N	VAL	A	507	21.692	30.784	0.417	1.00	32.90
ATOM	1639	CA	VAL	A	507	21.735	29.341	0.227	1.00	35.32
ATOM	1640	CB	VAL	A	507	20.809	28.932	-0.926	1.00	39.14
ATOM	1641	CG1	VAL	A	507	20.872	27.438	-1.155	1.00	41.89
ATOM	1642	CG2	VAL	A	507	19.382	29.364	-0.630	1.00	35.73
ATOM	1643	C	VAL	A	507	23.146	28.782	-0.016	1.00	35.01
ATOM	1644	O	VAL	A	507	23.447	27.642	0.318	1.00	36.47
ATOM	1645	N	SER	A	508	24.009	29.584	-0.616	1.00	36.29
ATOM	1646	CA	SER	A	508	25.372	29.159	-0.886	1.00	37.66
ATOM	1647	CB	SER	A	508	25.996	30.084	-1.941	1.00	38.93



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ATOM	1648	OG	SER	A	508	27.309	29.693	-2.294	1.00	45.66
ATOM	1649	C	SER	A	508	26.192	29.172	0.420	1.00	37.79
ATOM	1650	O	SER	A	508	27.026	28.280	0.647	1.00	37.44
ATOM	1651	N	THR	A	509	25.949	30.178	1.267	1.00	35.49
ATOM	1652	CA	THR	A	509	26.627	30.326	2.553	1.00	32.31
ATOM	1653	CB	THR	A	509	26.250	31.644	3.236	1.00	35.78
ATOM	1654	OG1	THR	A	509	26.405	32.720	2.305	1.00	42.43
ATOM	1655	CG2	THR	A	509	27.157	31.895	4.437	1.00	35.82
ATOM	1656	C	THR	A	509	26.231	29.187	3.469	1.00	28.28
ATOM	1657	O	THR	A	509	27.065	28.665	4.178	1.00	32.41
ATOM	1658	N	LEU	A	510	24.958	28.812	3.452	1.00	28.16
ATOM	1659	CA	LEU	A	510	24.452	27.696	4.249	1.00	29.00
ATOM	1660	CB	LEU	A	510	22.994	27.394	3.885	1.00	26.48
ATOM	1661	CG	LEU	A	510	21.819	28.079	4.571	1.00	29.80
ATOM	1662	CD1	LEU	A	510	20.544	27.623	3.907	1.00	28.25
ATOM	1663	CD2	LEU	A	510	21.793	27.717	6.063	1.00	30.36
ATOM	1664	C	LEU	A	510	25.267	26.437	3.969	1.00	32.43
ATOM	1665	O	LEU	A	510	25.639	25.698	4.885	1.00	32.33
ATOM	1666	N	ARG	A	511	25.524	26.194	2.685	1.00	31.40
ATOM	1667	CA	ARG	A	511	26.272	25.027	2.233	1.00	28.94
ATOM	1668	CB	ARG	A	511	26.170	24.909	0.706	1.00	34.59
ATOM	1669	CG	ARG	A	511	24.716	24.741	0.261	1.00	34.26
ATOM	1670	CD	ARG	A	511	24.547	24.611	-1.225	1.00	36.35
ATOM	1671	NE	ARG	A	511	23.192	24.185	-1.556	1.00	31.13
ATOM	1672	CZ	ARG	A	511	22.887	23.356	-2.545	1.00	31.68
ATOM	1673	NH1	ARG	A	511	23.839	22.856	-3.324	1.00	32.54
ATOM	1674	NH2	ARG	A	511	21.628	23.004	-2.730	1.00	27.68
ATOM	1675	C	ARG	A	511	27.710	25.049	2.695	1.00	26.34
ATOM	1676	O	ARG	A	511	28.270	24.011	3.015	1.00	28.74
ATOM	1677	N	ALA	A	512	28.314	26.235	2.693	1.00	25.39
ATOM	1678	CA	ALA	A	512	29.687	26.409	3.161	1.00	24.68
ATOM	1679	CB	ALA	A	512	30.157	27.796	2.830	1.00	22.96
ATOM	1680	C	ALA	A	512	29.732	26.195	4.691	1.00	27.69
ATOM	1681	O	ALA	A	512	30.622	25.518	5.231	1.00	27.18
ATOM	1682	N	LEU	A	513	28.773	26.814	5.373	1.00	27.16
ATOM	1683	CA	LEU	A	513	28.638	26.708	6.815	1.00	26.64
ATOM	1684	CB	LEU	A	513	27.427	27.528	7.256	1.00	24.45
ATOM	1685	CG	LEU	A	513	27.228	27.696	8.758	1.00	28.40
ATOM	1686	CD1	LEU	A	513	28.492	28.230	9.403	1.00	25.85
ATOM	1687	CD2	LEU	A	513	26.053	28.607	9.013	1.00	30.72
ATOM	1688	C	LEU	A	513	28.490	25.209	7.192	1.00	29.10
ATOM	1689	O	LEU	A	513	29.259	24.683	8.008	1.00	31.91
ATOM	1690	N	CYS	A	514	27.543	24.512	6.566	1.00	26.57
ATOM	1691	CA	CYS	A	514	27.351	23.104	6.851	1.00	26.98
ATOM	1692	CB	CYS	A	514	26.025	22.614	6.269	1.00	25.74
ATOM	1693	SG	CYS	A	514	24.579	23.438	7.009	1.00	30.96
ATOM	1694	C	CYS	A	514	28.538	22.250	6.404	1.00	28.07
ATOM	1695	O	CYS	A	514	28.764	21.161	6.931	1.00	27.30
ATOM	1696	N	GLY	A	515	29.298	22.741	5.431	1.00	29.78
ATOM	1697	CA	GLY	A	515	30.477	22.027	4.980	1.00	29.40
ATOM	1698	C	GLY	A	515	31.570	22.004	6.040	1.00	30.10
ATOM	1699	O	GLY	A	515	32.190	20.965	6.266	1.00	30.71
ATOM	1700	N	ARG	A	516	31.810	23.142	6.693	1.00	33.97
ATOM	1701	CA	ARG	A	516	32.811	23.217	7.748	1.00	34.03
ATOM	1702	CB	ARG	A	516	33.065	24.652	8.178	1.00	37.07
ATOM	1703	CG	ARG	A	516	33.921	25.429	7.198	1.00	52.01
ATOM	1704	CD	ARG	A	516	34.465	26.715	7.807	1.00	56.98
ATOM	1705	NE	ARG	A	516	35.467	26.438	8.836	1.00	61.64
ATOM	1706	CZ	ARG	A	516	35.927	27.342	9.699	1.00	62.65
ATOM	1707	NH1	ARG	A	516	35.466	28.590	9.665	1.00	61.40
ATOM	1708	NH2	ARG	A	516	36.879	27.005	10.566	1.00	60.38
ATOM	1709	C	ARG	A	516	32.380	22.395	8.947	1.00	33.89
ATOM	1710	O	ARG	A	516	33.227	21.847	9.634	1.00	33.31
ATOM	1711	N	HIS	A	517	31.075	22.322	9.215	1.00	33.19
ATOM	1712	CA	HIS	A	517	30.616	21.517	10.337	1.00	34.62
ATOM	1713	CB	HIS	A	517	29.085	21.466	10.440	1.00	34.29

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ATOM	1714	CG	HIS	A	517	28.576	20.462	11.440	1.00	33.44
ATOM	1715	CD2	HIS	A	517	28.646	20.433	12.793	1.00	31.33
ATOM	1716	ND1	HIS	A	517	27.909	19.311	11.072	1.00	28.67
ATOM	1717	CE1	HIS	A	517	27.589	18.619	12.151	1.00	27.08
ATOM	1718	NE2	HIS	A	517	28.027	19.279	13.208	1.00	28.43
ATOM	1719	C	HIS	A	517	31.147	20.107	10.127	1.00	36.73
ATOM	1720	O	HIS	A	517	31.825	19.567	10.994	1.00	34.74
ATOM	1721	N	THR	A	518	30.884	19.541	8.950	1.00	36.75
ATOM	1722	CA	THR	A	518	31.343	18.192	8.662	1.00	36.81
ATOM	1723	CB	THR	A	518	30.692	17.620	7.406	1.00	35.05
ATOM	1724	OG1	THR	A	518	29.327	17.303	7.688	1.00	37.15
ATOM	1725	CG2	THR	A	518	31.382	16.346	6.980	1.00	38.73
ATOM	1726	C	THR	A	518	32.862	18.100	8.608	1.00	37.39
ATOM	1727	O	THR	A	518	33.430	17.077	8.962	1.00	42.45
ATOM	1728	N	GLU	A	519	33.531	19.175	8.220	1.00	38.67
ATOM	1729	CA	GLU	A	519	34.990	19.166	8.196	1.00	43.58
ATOM	1730	CB	GLU	A	519	35.516	20.438	7.500	1.00	54.27
ATOM	1731	CG	GLU	A	519	35.261	20.537	5.964	1.00	63.20
ATOM	1732	CD	GLU	A	519	35.380	21.975	5.406	1.00	65.12
ATOM	1733	OE1	GLU	A	519	34.782	22.258	4.342	1.00	66.49
ATOM	1734	OE2	GLU	A	519	36.053	22.826	6.035	1.00	67.73
ATOM	1735	C	GLU	A	519	35.516	19.099	9.649	1.00	42.46
ATOM	1736	O	GLU	A	519	36.470	18.382	9.959	1.00	39.74
ATOM	1737	N	LYS	A	520	34.857	19.843	10.535	1.00	41.75
ATOM	1738	CA	LYS	A	520	35.222	19.895	11.945	1.00	37.07
ATOM	1739	CB	LYS	A	520	34.481	21.049	12.651	1.00	41.10
ATOM	1740	CG	LYS	A	520	34.939	22.467	12.235	1.00	44.66
ATOM	1741	CD	LYS	A	520	36.383	22.748	12.670	1.00	53.92
ATOM	1742	CE	LYS	A	520	37.078	23.819	11.819	1.00	56.95
ATOM	1743	NZ	LYS	A	520	37.313	23.411	10.388	1.00	63.31
ATOM	1744	C	LYS	A	520	34.911	18.560	12.618	1.00	34.80
ATOM	1745	O	LYS	A	520	35.770	17.983	13.278	1.00	34.89
ATOM	1746	N	LEU	A	521	33.703	18.051	12.394	1.00	33.45
ATOM	1747	CA	LEU	A	521	33.270	16.782	12.956	1.00	33.31
ATOM	1748	CB	LEU	A	521	31.839	16.460	12.526	1.00	26.37
ATOM	1749	CG	LEU	A	521	31.268	15.095	12.905	1.00	24.78
ATOM	1750	CD1	LEU	A	521	31.380	14.865	14.394	1.00	29.22
ATOM	1751	CD2	LEU	A	521	29.832	15.021	12.520	1.00	24.85
ATOM	1752	C	LEU	A	521	34.214	15.633	12.601	1.00	38.43
ATOM	1753	O	LEU	A	521	34.564	14.843	13.477	1.00	38.10
ATOM	1754	N	MET	A	522	34.694	15.581	11.356	1.00	39.97
ATOM	1755	CA	MET	A	522	35.601	14.507	10.947	1.00	41.97
ATOM	1756	CB	MET	A	522	35.725	14.431	9.426	1.00	48.01
ATOM	1757	CG	MET	A	522	34.430	14.035	8.707	1.00	58.55
ATOM	1758	SD	MET	A	522	33.355	12.804	9.548	1.00	67.62
ATOM	1759	CE	MET	A	522	34.455	11.351	9.732	1.00	65.55
ATOM	1760	C	MET	A	522	36.982	14.574	11.596	1.00	40.03
ATOM	1761	O	MET	A	522	37.578	13.539	11.900	1.00	37.83
ATOM	1762	N	ALA	A	523	37.497	15.782	11.798	1.00	37.94
ATOM	1763	CA	ALA	A	523	38.790	15.936	12.452	1.00	39.72
ATOM	1764	CB	ALA	A	523	39.272	17.353	12.304	1.00	45.50
ATOM	1765	C	ALA	A	523	38.640	15.587	13.938	1.00	41.81
ATOM	1766	O	ALA	A	523	39.523	14.997	14.547	1.00	44.06
ATOM	1767	N	PHE	A	524	37.509	15.971	14.519	1.00	41.49
ATOM	1768	CA	PHE	A	524	37.238	15.674	15.915	1.00	39.19
ATOM	1769	CB	PHE	A	524	35.923	16.334	16.360	1.00	35.12
ATOM	1770	CG	PHE	A	524	35.511	15.998	17.781	1.00	30.17
ATOM	1771	CD1	PHE	A	524	35.968	16.762	18.852	1.00	28.22
ATOM	1772	CD2	PHE	A	524	34.644	14.924	18.040	1.00	26.69
ATOM	1773	CE1	PHE	A	524	35.569	16.465	20.166	1.00	25.14
ATOM	1774	CE2	PHE	A	524	34.240	14.620	19.341	1.00	27.45
ATOM	1775	CZ	PHE	A	524	34.709	15.398	20.408	1.00	25.33
ATOM	1776	C	PHE	A	524	37.151	14.157	16.093	1.00	38.05
ATOM	1777	O	PHE	A	524	37.788	13.602	16.989	1.00	39.38
ATOM	1778	N	LYS	A	525	36.370	13.494	15.240	1.00	33.74
ATOM	1779	CA	LYS	A	525	36.188	12.053	15.336	1.00	32.28

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ATOM	1780	CB	LYS	A	525	35.150	11.566	14.341	1.00	32.43
ATOM	1781	CG	LYS	A	525	35.058	10.061	14.265	1.00	32.27
ATOM	1782	CD	LYS	A	525	34.049	9.588	13.234	1.00	39.70
ATOM	1783	CE	LYS	A	525	34.182	8.085	13.027	1.00	43.60
ATOM	1784	NZ	LYS	A	525	33.052	7.475	12.274	1.00	52.36
ATOM	1785	C	LYS	A	525	37.486	11.292	15.141	1.00	37.02
ATOM	1786	O	LYS	A	525	37.572	10.113	15.458	1.00	38.38
ATOM	1787	N	ALA	A	526	38.514	11.972	14.651	1.00	38.57
ATOM	1788	CA	ALA	A	526	39.796	11.312	14.442	1.00	42.31
ATOM	1789	CB	ALA	A	526	40.639	12.098	13.429	1.00	42.02
ATOM	1790	C	ALA	A	526	40.523	11.230	15.774	1.00	43.27
ATOM	1791	O	ALA	A	526	41.174	10.226	16.091	1.00	43.91
ATOM	1792	N	ILE	A	527	40.348	12.293	16.555	1.00	41.76
ATOM	1793	CA	ILE	A	527	40.961	12.455	17.866	1.00	40.21
ATOM	1794	CB	ILE	A	527	41.127	13.946	18.166	1.00	40.67
ATOM	1795	CG2	ILE	A	527	41.824	14.145	19.503	1.00	42.82
ATOM	1796	CG1	ILE	A	527	41.897	14.612	17.026	1.00	39.18
ATOM	1797	CD1	ILE	A	527	41.864	16.128	17.066	1.00	37.42
ATOM	1798	C	ILE	A	527	40.195	11.786	19.015	1.00	38.56
ATOM	1799	O	ILE	A	527	40.800	11.309	19.974	1.00	38.98
ATOM	1800	N	TYR	A	528	38.871	11.727	18.900	1.00	34.57
ATOM	1801	CA	TYR	A	528	38.023	11.135	19.930	1.00	31.38
ATOM	1802	CB	TYR	A	528	37.209	12.229	20.645	1.00	31.31
ATOM	1803	CG	TYR	A	528	38.046	13.379	21.159	1.00	34.92
ATOM	1804	CD1	TYR	A	528	38.337	14.471	20.345	1.00	34.80
ATOM	1805	CE1	TYR	A	528	39.157	15.513	20.789	1.00	39.08
ATOM	1806	CD2	TYR	A	528	38.592	13.355	22.442	1.00	34.45
ATOM	1807	CE2	TYR	A	528	39.417	14.394	22.895	1.00	37.74
ATOM	1808	CZ	TYR	A	528	39.695	15.468	22.062	1.00	39.56
ATOM	1809	OH	TYR	A	528	40.520	16.489	22.489	1.00	45.36
ATOM	1810	C	TYR	A	528	37.066	10.113	19.333	1.00	32.21
ATOM	1811	O	TYR	A	528	35.843	10.289	19.388	1.00	35.37
ATOM	1812	N	PRO	A	529	37.601	9.010	18.777	1.00	32.25
ATOM	1813	CD	PRO	A	529	39.034	8.705	18.673	1.00	29.41
ATOM	1814	CA	PRO	A	529	36.809	7.939	18.160	1.00	30.81
ATOM	1815	CB	PRO	A	529	37.875	6.895	17.822	1.00	30.02
ATOM	1816	CG	PRO	A	529	39.061	7.703	17.564	1.00	29.92
ATOM	1817	C	PRO	A	529	35.706	7.331	19.040	1.00	33.28
ATOM	1818	O	PRO	A	529	34.553	7.201	18.606	1.00	32.51
ATOM	1819	N	ASP	A	530	36.066	6.953	20.272	1.00	35.37
ATOM	1820	CA	ASP	A	530	35.110	6.338	21.195	1.00	35.88
ATOM	1821	CB	ASP	A	530	35.831	5.563	22.293	1.00	46.50
ATOM	1822	CG	ASP	A	530	36.564	4.341	21.758	1.00	58.80
ATOM	1823	OD1	ASP	A	530	36.010	3.219	21.852	1.00	64.43
ATOM	1824	OD2	ASP	A	530	37.697	4.503	21.240	1.00	63.77
ATOM	1825	C	ASP	A	530	34.127	7.309	21.799	1.00	29.27
ATOM	1826	O	ASP	A	530	33.037	6.909	22.221	1.00	29.58
ATOM	1827	N	ILE	A	531	34.525	8.577	21.892	1.00	30.58
ATOM	1828	CA	ILE	A	531	33.629	9.593	22.426	1.00	29.77
ATOM	1829	CB	ILE	A	531	34.302	10.998	22.576	1.00	35.01
ATOM	1830	CG2	ILE	A	531	33.230	12.090	22.817	1.00	33.87
ATOM	1831	CG1	ILE	A	531	35.247	10.998	23.781	1.00	36.43
ATOM	1832	CD1	ILE	A	531	34.549	10.604	25.107	1.00	36.43
ATOM	1833	C	ILE	A	531	32.500	9.673	21.440	1.00	29.02
ATOM	1834	O	ILE	A	531	31.344	9.560	21.819	1.00	33.33
ATOM	1835	N	VAL	A	532	32.841	9.787	20.158	1.00	29.79
ATOM	1836	CA	VAL	A	532	31.814	9.857	19.129	1.00	25.98
ATOM	1837	CB	VAL	A	532	32.446	10.141	17.746	1.00	27.17
ATOM	1838	CG1	VAL	A	532	31.376	10.244	16.699	1.00	26.57
ATOM	1839	CG2	VAL	A	532	33.246	11.437	17.788	1.00	23.54
ATOM	1840	C	VAL	A	532	30.984	8.567	19.111	1.00	22.88
ATOM	1841	O	VAL	A	532	29.765	8.596	19.258	1.00	25.44
ATOM	1842	N	ARG	A	533	31.662	7.429	19.048	1.00	24.52
ATOM	1843	CA	ARG	A	533	30.980	6.136	18.997	1.00	23.99
ATOM	1844	CB	ARG	A	533	32.028	5.030	18.941	1.00	28.41
ATOM	1845	CG	ARG	A	533	31.444	3.657	18.777	1.00	37.43

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ATOM	1846	CD	ARG	A	533	32.551	2.627	18.668	1.00	45.29
ATOM	1847	NE	ARG	A	533	32.255	1.490	19.528	1.00	51.73
ATOM	1848	CZ	ARG	A	533	32.897	1.228	20.658	1.00	55.49
ATOM	1849	NH1	ARG	A	533	33.899	2.010	21.052	1.00	51.92
ATOM	1850	NH2	ARG	A	533	32.459	0.254	21.445	1.00	59.77
ATOM	1851	C	ARG	A	533	30.024	5.861	20.136	1.00	24.93
ATOM	1852	O	ARG	A	533	28.866	5.504	19.935	1.00	24.06
ATOM	1853	N	LEU	A	534	30.519	6.093	21.348	1.00	30.94
ATOM	1854	CA	LEU	A	534	29.778	5.846	22.582	1.00	26.49
ATOM	1855	CB	LEU	A	534	30.773	5.408	23.658	1.00	28.50
ATOM	1856	CG	LEU	A	534	31.461	4.072	23.339	1.00	28.71
ATOM	1857	CD1	LEU	A	534	32.692	3.806	24.193	1.00	29.88
ATOM	1858	CD2	LEU	A	534	30.436	2.985	23.497	1.00	29.34
ATOM	1859	C	LEU	A	534	28.877	6.956	23.118	1.00	24.89
ATOM	1860	O	LEU	A	534	27.803	6.669	23.649	1.00	24.01
ATOM	1861	N	HIS	A	535	29.234	8.214	22.875	1.00	25.63
ATOM	1862	CA	HIS	A	535	28.458	9.317	23.439	1.00	27.16
ATOM	1863	CB	HIS	A	535	29.358	10.074	24.423	1.00	26.58
ATOM	1864	CG	HIS	A	535	30.001	9.174	25.430	1.00	25.50
ATOM	1865	CD2	HIS	A	535	31.245	8.641	25.487	1.00	25.11
ATOM	1866	ND1	HIS	A	535	29.302	8.631	26.487	1.00	26.41
ATOM	1867	CE1	HIS	A	535	30.086	7.802	27.151	1.00	24.19
ATOM	1868	NE2	HIS	A	535	31.270	7.790	26.564	1.00	26.77
ATOM	1869	C	HIS	A	535	27.669	10.284	22.553	1.00	28.58
ATOM	1870	O	HIS	A	535	26.881	11.073	23.082	1.00	27.81
ATOM	1871	N	PHE	A	536	27.851	10.228	21.226	1.00	33.00
ATOM	1872	CA	PHE	A	536	27.092	11.108	20.313	1.00	31.11
ATOM	1873	CB	PHE	A	536	27.895	11.401	19.043	1.00	29.90
ATOM	1874	CG	PHE	A	536	28.915	12.512	19.192	1.00	29.99
ATOM	1875	CD1	PHE	A	536	29.678	12.643	20.337	1.00	24.61
ATOM	1876	CD2	PHE	A	536	29.132	13.406	18.153	1.00	25.96
ATOM	1877	CE1	PHE	A	536	30.644	13.642	20.439	1.00	23.54
ATOM	1878	CE2	PHE	A	536	30.095	14.406	18.256	1.00	24.50
ATOM	1879	CZ	PHE	A	536	30.849	14.523	19.394	1.00	24.21
ATOM	1880	C	PHE	A	536	25.713	10.487	19.970	1.00	31.08
ATOM	1881	O	PHE	A	536	25.581	9.259	19.956	1.00	34.36
ATOM	1882	N	PRO	A	537	24.664	11.321	19.756	1.00	27.00
ATOM	1883	CD	PRO	A	537	24.632	12.793	19.845	1.00	25.60
ATOM	1884	CA	PRO	A	537	23.335	10.795	19.432	1.00	25.30
ATOM	1885	CB	PRO	A	537	22.501	12.068	19.256	1.00	23.10
ATOM	1886	CG	PRO	A	537	23.189	13.062	20.157	1.00	22.43
ATOM	1887	C	PRO	A	537	23.392	9.975	18.128	1.00	30.48
ATOM	1888	O	PRO	A	537	24.122	10.336	17.185	1.00	28.64
ATOM	1889	N	PRO	A	538	22.690	8.823	18.091	1.00	31.20
ATOM	1890	CD	PRO	A	538	22.017	8.173	19.227	1.00	28.91
ATOM	1891	CA	PRO	A	538	22.654	7.946	16.908	1.00	32.16
ATOM	1892	CB	PRO	A	538	21.592	6.931	17.293	1.00	29.35
ATOM	1893	CG	PRO	A	538	21.911	6.731	18.759	1.00	28.32
ATOM	1894	C	PRO	A	538	22.311	8.708	15.623	1.00	32.64
ATOM	1895	O	PRO	A	538	23.086	8.680	14.669	1.00	30.42
ATOM	1896	N	LEU	A	539	21.207	9.460	15.652	1.00	34.18
ATOM	1897	CA	LEU	A	539	20.773	10.273	14.510	1.00	30.02
ATOM	1898	CB	LEU	A	539	19.512	11.069	14.895	1.00	29.47
ATOM	1899	CG	LEU	A	539	18.858	11.924	13.802	1.00	29.66
ATOM	1900	CD1	LEU	A	539	18.592	11.029	12.608	1.00	31.73
ATOM	1901	CD2	LEU	A	539	17.583	12.604	14.267	1.00	25.29
ATOM	1902	C	LEU	A	539	21.887	11.215	14.009	1.00	29.19
ATOM	1903	O	LEU	A	539	22.131	11.326	12.816	1.00	30.25
ATOM	1904	N	TYR	A	540	22.581	11.877	14.925	1.00	25.32
ATOM	1905	CA	TYR	A	540	23.643	12.778	14.546	1.00	22.42
ATOM	1906	CB	TYR	A	540	24.280	13.355	15.791	1.00	21.19
ATOM	1907	CG	TYR	A	540	25.343	14.387	15.535	1.00	17.26
ATOM	1908	CD1	TYR	A	540	25.016	15.733	15.400	1.00	17.30
ATOM	1909	CE1	TYR	A	540	25.982	16.676	15.216	1.00	12.79
ATOM	1910	CD2	TYR	A	540	26.680	14.028	15.464	1.00	19.93
ATOM	1911	CE2	TYR	A	540	27.657	14.976	15.268	1.00	20.13

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ATOM	1912	CZ	TYR	A	540	27.294	16.299	15.150	1.00	13.88
ATOM	1913	OH	TYR	A	540	28.276	17.244	14.997	1.00	21.75
ATOM	1914	C	TYR	A	540	24.708	12.009	13.780	1.00	32.70
ATOM	1915	O	TYR	A	540	25.296	12.508	12.811	1.00	34.57
ATOM	1916	N	LYS	A	541	25.008	10.802	14.244	1.00	35.66
ATOM	1917	CA	LYS	A	541	26.029	9.999	13.574	1.00	36.65
ATOM	1918	CB	LYS	A	541	26.482	8.874	14.497	1.00	32.71
ATOM	1919	CG	LYS	A	541	27.219	9.383	15.714	1.00	31.67
ATOM	1920	CD	LYS	A	541	27.712	8.227	16.528	1.00	26.84
ATOM	1921	CE	LYS	A	541	26.561	7.418	17.035	1.00	22.56
ATOM	1922	NZ	LYS	A	541	27.091	6.148	17.574	1.00	31.19
ATOM	1923	C	LYS	A	541	25.563	9.467	12.204	1.00	32.35
ATOM	1924	O	LYS	A	541	26.324	9.441	11.250	1.00	34.75
ATOM	1925	N	GLU	A	542	24.298	9.069	12.126	1.00	32.04
ATOM	1926	CA	GLU	A	542	23.726	8.570	10.888	1.00	35.69
ATOM	1927	CB	GLU	A	542	22.316	8.074	11.129	1.00	38.46
ATOM	1928	CG	GLU	A	542	22.269	6.772	11.888	1.00	52.51
ATOM	1929	CD	GLU	A	542	20.882	6.443	12.403	1.00	59.88
ATOM	1930	OE1	GLU	A	542	20.795	5.892	13.531	1.00	65.14
ATOM	1931	OE2	GLU	A	542	19.889	6.732	11.684	1.00	59.01
ATOM	1932	C	GLU	A	542	23.661	9.668	9.855	1.00	36.75
ATOM	1933	O	GLU	A	542	23.668	9.393	8.666	1.00	39.22
ATOM	1934	N	LEU	A	543	23.557	10.913	10.312	1.00	35.21
ATOM	1935	CA	LEU	A	543	23.449	12.047	9.407	1.00	33.98
ATOM	1936	CB	LEU	A	543	22.549	13.145	9.990	1.00	31.70
ATOM	1937	CG	LEU	A	543	21.045	12.927	10.118	1.00	34.06
ATOM	1938	CD1	LEU	A	543	20.457	14.088	10.891	1.00	35.24
ATOM	1939	CD2	LEU	A	543	20.388	12.826	8.761	1.00	35.42
ATOM	1940	C	LEU	A	543	24.731	12.702	8.959	1.00	32.29
ATOM	1941	O	LEU	A	543	24.776	13.231	7.859	1.00	39.03
ATOM	1942	N	PHE	A	544	25.781	12.651	9.762	1.00	29.28
ATOM	1943	CA	PHE	A	544	26.997	13.354	9.389	1.00	29.14
ATOM	1944	CB	PHE	A	544	27.203	14.561	10.330	1.00	32.64
ATOM	1945	CG	PHE	A	544	25.969	15.425	10.528	1.00	32.31
ATOM	1946	CD1	PHE	A	544	25.295	15.431	11.746	1.00	27.53
ATOM	1947	CD2	PHE	A	544	25.491	16.247	9.501	1.00	32.38
ATOM	1948	CE1	PHE	A	544	24.165	16.239	11.943	1.00	26.56
ATOM	1949	CE2	PHE	A	544	24.354	17.065	9.690	1.00	29.30
ATOM	1950	CZ	PHE	A	544	23.694	17.057	10.914	1.00	30.03
ATOM	1951	C	PHE	A	544	28.269	12.505	9.356	1.00	33.29
ATOM	1952	O	PHE	A	544	28.193	11.266	9.571	1.00	36.40
ATOM	1953	OXT	PHE	A	544	29.349	13.102	9.110	1.00	34.60
ATOM	1954	O1	HOH	V	1	19.571	24.015	22.830	1.00	11.92
ATOM	1955	O1	HOH	V	2	12.600	24.091	16.912	1.00	16.18
ATOM	1956	O1	HOH	V	3	14.052	22.894	14.638	1.00	22.41
ATOM	1957	O1	HOH	V	4	28.663	16.841	27.507	1.00	23.15
ATOM	1958	O1	HOH	V	5	26.725	9.526	26.728	1.00	24.50
ATOM	1959	O1	HOH	V	6	18.179	21.587	21.082	1.00	24.52
ATOM	1960	O1	HOH	V	7	34.584	18.654	31.591	1.00	24.62
ATOM	1961	O1	HOH	V	8	38.207	8.705	22.227	1.00	25.07
ATOM	1962	O1	HOH	V	9	18.077	19.002	0.819	1.00	25.07
ATOM	1963	O1	HOH	V	10	17.420	26.679	24.799	1.00	25.52
ATOM	1964	O1	HOH	V	11	11.110	25.828	9.180	1.00	25.56
ATOM	1965	O1	HOH	V	12	25.371	34.354	26.992	1.00	25.89
ATOM	1966	O1	HOH	V	13	35.321	27.213	19.620	1.00	25.99
ATOM	1967	O1	HOH	V	14	18.045	26.166	21.645	1.00	26.14
ATOM	1968	O1	HOH	V	15	19.454	10.080	17.919	1.00	26.31
ATOM	1969	O1	HOH	V	16	37.357	26.490	13.415	1.00	26.89
ATOM	1970	O1	HOH	V	17	11.508	26.772	18.302	1.00	27.31
ATOM	1971	O1	HOH	V	18	15.147	25.780	21.426	1.00	27.73
ATOM	1972	O1	HOH	V	19	26.400	37.545	37.765	1.00	27.84
ATOM	1973	O1	HOH	V	20	24.927	38.184	32.702	1.00	28.88
ATOM	1974	O1	HOH	V	21	22.535	18.724	7.093	1.00	29.31
ATOM	1975	O1	HOH	V	22	19.050	8.455	-3.987	1.00	29.80
ATOM	1976	O1	HOH	V	23	20.732	38.540	24.291	1.00	30.07
ATOM	1977	O1	HOH	V	24	14.054	28.783	15.745	1.00	31.20

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ATOM	1978	01	HOH	V	25	25.356	15.005	28.051	1.00	31.83
ATOM	1979	01	HOH	V	26	33.279	26.348	25.938	1.00	32.16
ATOM	1980	01	HOH	V	27	14.590	28.615	28.744	1.00	32.70
ATOM	1981	01	HOH	V	28	4.102	35.198	9.164	1.00	32.70
ATOM	1982	01	HOH	V	29	13.577	30.615	29.768	1.00	32.70
ATOM	1983	01	HOH	V	30	28.564	37.851	14.236	1.00	32.76
ATOM	1984	01	HOH	V	31	22.927	14.143	0.962	1.00	33.39
ATOM	1985	01	HOH	V	32	27.550	38.081	22.254	1.00	33.51
ATOM	1986	01	HOH	V	33	4.343	30.099	9.792	1.00	33.68
ATOM	1987	01	HOH	V	34	13.758	27.478	19.451	1.00	33.73
ATOM	1988	01	HOH	V	35	31.045	36.851	16.729	1.00	33.87
ATOM	1989	01	HOH	V	36	19.213	14.762	21.135	1.00	33.94
ATOM	1990	01	HOH	V	37	30.260	38.889	20.375	1.00	34.05
ATOM	1991	01	HOH	V	38	21.211	20.354	29.122	1.00	34.10
ATOM	1992	01	HOH	V	39	32.966	5.622	27.344	1.00	34.62
ATOM	1993	01	HOH	V	40	26.116	6.668	20.629	1.00	35.56
ATOM	1994	01	HOH	V	41	-1.516	28.517	7.655	1.00	35.63
ATOM	1995	01	HOH	V	42	34.189	32.470	17.850	1.00	35.68
ATOM	1996	01	HOH	V	43	24.220	21.292	3.001	1.00	35.74
ATOM	1997	01	HOH	V	44	5.910	27.836	16.119	1.00	36.07
ATOM	1998	01	HOH	V	45	26.026	15.360	5.513	1.00	36.54
ATOM	1999	01	HOH	V	46	24.021	14.774	-1.204	1.00	36.65
ATOM	2000	01	HOH	V	47	20.363	26.930	31.179	1.00	36.70
ATOM	2001	01	HOH	V	48	35.665	32.840	10.425	1.00	36.70
ATOM	2002	01	HOH	V	49	26.360	37.660	34.946	1.00	36.83
ATOM	2003	01	HOH	V	50	25.128	17.207	-1.881	1.00	36.96
ATOM	2004	01	HOH	V	51	24.114	21.504	30.329	1.00	37.03
ATOM	2005	01	HOH	V	52	15.366	43.743	10.778	1.00	37.39
ATOM	2006	01	HOH	V	53	30.933	6.183	15.530	1.00	37.82
ATOM	2007	01	HOH	V	54	4.304	36.868	5.949	1.00	38.21
ATOM	2008	01	HOH	V	55	14.763	35.710	19.412	1.00	39.01
ATOM	2009	01	HOH	V	56	1.357	20.195	9.921	1.00	39.03
ATOM	2010	01	HOH	V	57	13.913	23.892	19.724	1.00	39.09
ATOM	2011	01	HOH	V	58	12.354	12.577	-11.744	1.00	39.57
ATOM	2012	01	HOH	V	59	19.367	4.873	15.945	1.00	39.60
ATOM	2013	01	HOH	V	60	28.823	27.044	-1.138	1.00	39.87
ATOM	2014	01	HOH	V	61	24.086	5.629	14.333	1.00	39.92
ATOM	2015	01	HOH	V	62	6.227	36.542	12.153	1.00	39.94
ATOM	2016	01	HOH	V	63	25.257	19.031	30.271	1.00	40.01
ATOM	2017	01	HOH	V	64	33.091	35.051	17.676	1.00	40.07
ATOM	2018	01	HOH	V	65	33.832	31.154	20.549	1.00	40.37
ATOM	2019	01	HOH	V	66	40.477	15.296	9.510	1.00	41.20
ATOM	2020	01	HOH	V	67	23.525	9.325	-8.918	1.00	41.87
ATOM	2021	01	HOH	V	68	18.624	25.089	-4.128	1.00	42.15
ATOM	2022	01	HOH	V	69	24.673	39.002	-1.542	1.00	42.21
ATOM	2023	01	HOH	V	70	25.134	15.085	2.723	1.00	42.21
ATOM	2024	01	HOH	V	71	10.336	29.797	26.075	1.00	42.37
ATOM	2025	01	HOH	V	72	16.798	18.655	-11.711	1.00	42.43
ATOM	2026	01	HOH	V	73	-2.391	33.028	0.604	1.00	42.69
ATOM	2027	01	HOH	V	74	7.033	20.764	20.270	1.00	43.01
ATOM	2028	01	HOH	V	75	27.375	26.586	32.414	1.00	43.08
ATOM	2029	01	HOH	V	76	24.651	12.458	27.335	1.00	43.14
ATOM	2030	01	HOH	V	77	21.223	24.850	0.260	1.00	43.31
ATOM	2031	01	HOH	V	78	13.059	10.272	13.532	1.00	43.63
ATOM	2032	01	HOH	V	79	27.284	19.103	8.210	1.00	44.00
ATOM	2033	01	HOH	V	80	34.897	34.595	21.757	1.00	44.35
ATOM	2034	01	HOH	V	81	19.496	24.289	-1.468	1.00	44.41
ATOM	2035	01	HOH	V	82	26.589	22.429	32.257	1.00	44.58
ATOM	2036	01	HOH	V	83	41.875	11.753	22.776	1.00	44.72
ATOM	2037	01	HOH	V	84	24.041	16.824	29.300	1.00	44.91
ATOM	2038	01	HOH	V	85	39.182	23.600	24.591	1.00	45.03
ATOM	2039	01	HOH	V	86	16.711	29.367	31.469	1.00	45.22
ATOM	2040	01	HOH	V	87	26.474	37.247	27.330	1.00	45.42
ATOM	2041	01	HOH	V	88	10.580	10.952	7.001	1.00	45.46
ATOM	2042	01	HOH	V	89	17.919	17.134	23.482	1.00	45.53
ATOM	2043	01	HOH	V	90	22.700	27.169	33.013	1.00	45.86

ATOM	2044	01	HOH	V	91	20.218	40.609	29.025	1.00	46.30
ATOM	2045	01	HOH	V	92	21.955	40.569	26.103	1.00	46.31
ATOM	2046	01	HOH	V	93	5.333	26.234	18.852	1.00	46.91
ATOM	2047	01	HOH	V	94	6.403	18.038	15.920	1.00	47.12
ATOM	2048	01	HOH	V	95	37.307	11.015	10.807	1.00	47.31
ATOM	2049	01	HOH	V	96	11.338	13.464	13.985	1.00	47.96
ATOM	2050	01	HOH	V	97	10.441	37.707	30.346	1.00	48.02
ATOM	2051	01	HOH	V	98	30.888	36.428	14.084	1.00	48.48
ATOM	2052	01	HOH	V	99	27.882	17.980	29.841	1.00	48.50
ATOM	2053	01	HOH	V	100	33.749	37.917	8.734	1.00	48.51
ATOM	2054	01	HOH	V	101	18.379	27.870	33.046	1.00	48.64
ATOM	2055	01	HOH	V	102	35.449	31.668	8.141	1.00	48.94
ATOM	2056	01	HOH	V	103	29.164	17.601	3.576	1.00	49.29
ATOM	2057	01	HOH	V	104	33.653	32.899	6.888	1.00	49.36
ATOM	2058	01	HOH	V	105	42.507	15.827	13.475	1.00	49.69
ATOM	2059	01	HOH	V	106	37.222	20.712	33.061	1.00	49.71
ATOM	2060	01	HOH	V	107	19.173	42.140	26.556	1.00	49.87
ATOM	2061	01	HOH	V	108	-1.128	28.133	10.338	1.00	50.07
ATOM	2062	01	HOH	V	109	13.605	40.750	25.634	1.00	50.16
ATOM	2063	01	HOH	V	110	-1.457	28.059	-4.001	1.00	50.19
ATOM	2064	01	HOH	V	111	-0.092	31.118	6.416	1.00	50.25
ATOM	2065	01	HOH	V	112	3.374	39.612	-3.935	1.00	50.31
ATOM	2066	01	HOH	V	113	32.127	18.267	32.763	1.00	50.37
ATOM	2067	01	HOH	V	114	18.258	23.101	26.041	1.00	50.51
ATOM	2068	01	HOH	V	115	26.516	26.089	-3.694	1.00	50.63
ATOM	2069	01	HOH	V	116	13.352	17.048	19.784	1.00	50.83
ATOM	2070	01	HOH	V	117	10.647	6.108	12.167	1.00	50.93
ATOM	2071	01	HOH	V	118	26.146	17.547	1.891	1.00	50.94
ATOM	2072	01	HOH	V	119	15.203	21.870	20.133	1.00	50.98
ATOM	2073	01	HOH	V	120	32.029	18.786	4.116	1.00	51.10
ATOM	2074	01	HOH	V	121	22.114	18.269	27.109	1.00	51.46
ATOM	2075	01	HOH	V	122	25.668	18.396	5.657	1.00	51.52
ATOM	2076	01	HOH	V	123	41.989	18.102	20.145	1.00	51.77
ATOM	2077	01	HOH	V	124	36.078	5.753	14.297	1.00	52.16
ATOM	2078	01	HOH	V	125	-4.191	23.385	-0.546	1.00	52.19
ATOM	2079	01	HOH	V	126	38.840	23.465	28.263	1.00	52.44
ATOM	2080	01	HOH	V	127	17.889	40.107	16.024	1.00	52.46
ATOM	2081	01	HOH	V	128	10.480	31.213	29.646	1.00	52.47
ATOM	2082	01	HOH	V	129	11.041	40.539	4.064	1.00	52.63
ATOM	2083	01	HOH	V	130	25.662	37.407	30.124	1.00	52.65
ATOM	2084	01	HOH	V	131	37.583	19.513	14.379	1.00	52.79
ATOM	2085	01	HOH	V	132	31.355	36.654	28.009	1.00	52.82
ATOM	2086	01	HOH	V	133	24.495	25.685	32.162	1.00	52.92
ATOM	2087	01	HOH	V	134	29.710	0.923	19.113	1.00	52.92
ATOM	2088	01	HOH	V	135	17.608	9.016	9.185	1.00	52.96
ATOM	2089	01	HOH	V	136	24.883	4.742	16.973	1.00	53.32
ATOM	2090	01	HOH	V	137	29.325	41.144	15.563	1.00	54.00
ATOM	2091	01	HOH	V	138	8.148	32.691	27.089	1.00	54.14
ATOM	2092	01	HOH	V	139	25.869	44.302	17.088	1.00	54.60
ATOM	2093	01	HOH	V	140	31.180	24.098	0.471	1.00	54.96
ATOM	2094	01	HOH	V	141	32.092	39.604	16.380	1.00	55.48
ATOM	2095	01	HOH	V	142	20.031	28.982	35.641	1.00	55.95
ATOM	2096	01	HOH	V	143	19.537	17.716	26.209	1.00	56.58
ATOM	2097	01	HOH	V	144	3.004	26.615	21.765	1.00	56.65
ATOM	2098	01	HOH	V	145	3.566	13.601	10.033	1.00	56.98
ATOM	2099	01	HOH	V	146	16.090	48.803	-0.839	1.00	57.02
ATOM	2100	01	HOH	V	147	41.521	30.957	16.321	1.00	57.24
ATOM	2101	01	HOH	V	148	21.322	6.331	6.002	1.00	57.58
ATOM	2102	01	HOH	V	149	9.375	39.538	12.218	1.00	57.59
ATOM	2103	01	HOH	V	150	15.176	39.661	18.686	1.00	58.07
ATOM	2104	01	HOH	V	151	20.363	24.179	31.362	1.00	58.21
ATOM	2105	01	HOH	V	152	14.157	40.583	21.313	1.00	58.26
ATOM	2106	01	HOH	V	153	13.420	36.512	16.363	1.00	58.51
ATOM	2107	01	HOH	V	154	1.911	36.126	4.549	1.00	58.55
ATOM	2108	01	HOH	V	155	16.108	6.884	12.075	1.00	58.70
ATOM	2109	01	HOH	V	156	-4.815	29.631	-4.704	1.00	58.74

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ATOM	2110	01	HOH V	157	17.728	4.118	0.882	1.00	59.17
ATOM	2111	01	HOH V	158	11.034	33.423	31.437	1.00	59.38
ATOM	2112	01	HOH V	159	39.277	19.752	9.565	1.00	59.80
ATOM	2113	01	HOH V	160	20.830	23.224	-9.945	1.00	59.89
ATOM	2114	01	HOH V	161	29.709	18.612	31.510	1.00	60.09
ATOM	2115	01	HOH V	162	27.074	2.621	20.642	1.00	60.12
ATOM	2116	01	HOH V	163	5.858	22.161	-4.489	1.00	60.19
ATOM	2117	01	HOH V	164	15.034	44.034	5.590	1.00	60.39
ATOM	2118	01	HOH V	165	33.009	22.978	33.387	1.00	60.43
ATOM	2119	01	HOH V	166	2.030	21.719	-4.397	1.00	60.59
ATOM	2120	01	HOH V	167	3.774	21.532	3.731	1.00	60.68
ATOM	2121	01	HOH V	168	28.412	13.665	-7.177	1.00	60.83
ATOM	2122	01	HOH V	169	39.061	22.162	31.337	1.00	61.22
ATOM	2123	01	HOH V	170	30.385	11.086	11.347	1.00	61.45
ATOM	2124	01	HOH V	171	38.929	11.728	26.423	1.00	61.62
ATOM	2125	01	HOH V	172	9.596	6.343	-6.409	1.00	61.85
ATOM	2126	01	HOH V	173	27.960	21.516	2.108	1.00	61.90
ATOM	2127	01	HOH V	174	4.313	13.515	-0.097	1.00	62.15
ATOM	2128	01	HOH V	175	-4.186	27.811	7.260	1.00	62.60
ATOM	2129	01	HOH V	176	10.940	41.489	27.508	1.00	63.29
ATOM	2130	01	HOH V	177	24.701	19.822	-1.623	1.00	63.64
ATOM	2131	01	HOH V	178	42.644	18.535	10.330	1.00	63.68
ATOM	2132	01	HOH V	179	1.986	36.706	26.540	1.00	63.68
ATOM	2133	01	HOH V	180	22.345	47.189	18.548	1.00	64.72
ATOM	2134	01	HOH V	181	7.492	6.994	1.249	1.00	64.77
ATOM	2135	01	HOH V	182	29.348	37.819	26.783	1.00	64.90
ATOM	2136	01	HOH V	183	39.883	20.258	25.832	1.00	65.05
ATOM	2137	01	HOH V	184	33.197	24.977	3.656	1.00	65.28
ATOM	2138	01	HOH V	185	1.167	34.045	3.205	1.00	65.41
ATOM	2139	01	HOH V	186	36.275	32.735	23.649	1.00	65.48
ATOM	2140	01	HOH V	187	-2.787	30.904	-0.828	1.00	65.58
ATOM	2141	01	HOH V	188	6.538	23.682	-10.695	1.00	66.34
ATOM	2142	01	HOH V	189	10.682	8.724	11.380	1.00	66.87
ATOM	2143	01	HOH V	190	14.198	8.869	-12.442	1.00	67.21
ATOM	2144	01	HOH V	191	-2.267	38.672	-2.479	1.00	67.22
ATOM	2145	01	HOH V	192	29.224	8.950	12.107	1.00	67.30
ATOM	2146	01	HOH V	193	11.819	8.883	6.281	1.00	67.62
ATOM	2147	01	HOH V	194	38.489	16.915	8.462	1.00	68.36
ATOM	2148	01	HOH V	195	33.987	7.482	15.967	1.00	68.84
ATOM	2149	01	HOH V	196	4.892	34.328	-7.351	1.00	68.88
ATOM	2150	01	HOH V	197	39.056	27.510	8.823	1.00	68.92
ATOM	2151	01	HOH V	198	9.884	6.802	3.712	1.00	69.08
ATOM	2152	01	HOH V	199	37.843	34.495	12.256	1.00	69.20
ATOM	2153	01	HOH V	200	34.349	36.343	19.667	1.00	69.76
ATOM	2154	01	HOH V	201	38.474	1.028	20.411	1.00	70.03
ATOM	2155	01	HOH V	202	27.053	38.768	25.134	1.00	70.09
ATOM	2156	01	HOH V	203	28.267	37.799	29.494	1.00	70.65
ATOM	2157	01	HOH V	204	25.427	35.915	1.694	1.00	71.85
ATOM	2158	01	HOH V	205	18.375	3.341	9.734	1.00	72.08
ATOM	2159	01	HOH V	206	29.055	24.527	-1.260	1.00	72.11
ATOM	2160	01	HOH V	207	15.436	3.667	-5.477	1.00	72.50
ATOM	2161	01	HOH V	208	2.845	25.343	17.594	1.00	72.71
ATOM	2162	01	HOH V	209	31.127	39.615	33.793	1.00	74.83
ATOM	2163	01	HOH V	210	15.559	12.402	-12.936	1.00	75.70
ATOM	2164	01	HOH V	211	40.158	26.133	22.103	1.00	76.15
ATOM	2165	01	HOH V	212	3.811	32.891	15.563	1.00	77.51
ATOM	2166	01	HOH V	213	21.251	45.356	7.011	1.00	78.54
ATOM	2167	01	HOH V	214	31.582	39.863	24.269	1.00	79.14
ATOM	2168	01	HOH V	215	-0.088	20.677	7.373	1.00	79.61
ATOM	2169	01	HOH V	216	34.466	33.712	35.188	1.00	80.04
ATOM	2170	01	HOH V	217	5.299	14.605	2.187	1.00	82.20
ATOM	2171	01	HOH V	218	-0.119	43.183	-1.190	1.00	82.43
ATOM	2172	01	HOH V	219	21.612	10.359	-10.786	1.00	83.22
ATOM	2173	01	HOH V	220	18.145	42.688	23.379	1.00	83.87
ATOM	2174	01	HOH V	221	38.141	26.882	26.796	1.00	84.27
ATOM	2175	01	HOH V	222	15.645	37.869	15.459	1.00	86.80



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ATOM	2176	O1	HOH	V	223	33.347	0.052	24.088	1.00	88.51
ATOM	2177	O1	HOH	V	224	26.717	9.812	6.181	1.00	89.08
ATOM	2178	O1	HOH	V	225	13.496	7.603	15.584	1.00	89.47
ATOM	2179	O1	HOH	V	226	0.897	31.611	9.140	1.00	89.58
ATOM	2180	O1	HOH	V	227	13.018	26.525	-7.628	1.00	90.92
ATOM	2181	O1	HOH	V	228	6.286	19.849	17.755	1.00	91.50
ATOM	2182	O1	HOH	V	229	19.825	7.712	0.669	1.00	92.59
ATOM	2183	O1	HOH	V	230	16.141	11.181	20.218	1.00	93.48
ATOM	2184	O1	HOH	V	231	30.341	41.381	18.146	1.00	94.31
ATOM	2185	C1	CHO	L	1	18.565	26.648	16.097	1.00	17.77
ATOM	2186	C4	CHO	L	1	17.062	26.995	16.208	1.00	14.30
ATOM	2187	C7	CHO	L	1	16.300	25.791	16.806	1.00	16.71
ATOM	2188	C9	CHO	L	1	16.836	25.493	18.221	1.00	17.53
ATOM	2189	C12	CHO	L	1	18.329	25.274	18.190	1.00	21.09
ATOM	2190	C13	CHO	L	1	18.814	24.179	18.791	1.00	17.61
ATOM	2191	C15	CHO	L	1	20.283	23.851	18.848	1.00	16.99
ATOM	2192	C18	CHO	L	1	21.159	25.087	18.576	1.00	18.07
ATOM	2193	C20	CHO	L	1	20.643	25.806	17.292	1.00	18.92
ATOM	2194	C22	CHO	L	1	19.182	26.326	17.485	1.00	20.91
ATOM	2195	C23	CHO	L	1	21.613	26.937	16.851	1.00	19.33
ATOM	2196	C26	CHO	L	1	23.077	26.440	16.727	1.00	23.26
ATOM	2197	C29	CHO	L	1	23.552	25.816	18.063	1.00	24.98
ATOM	2198	C30	CHO	L	1	22.616	24.628	18.351	1.00	19.40
ATOM	2199	C32	CHO	L	1	23.316	23.866	19.486	1.00	18.81
ATOM	2200	C35	CHO	L	1	24.818	24.074	19.179	1.00	18.34
ATOM	2201	C38	CHO	L	1	24.905	25.059	17.980	1.00	20.78
ATOM	2202	C40	CHO	L	1	23.518	26.864	19.214	1.00	25.58
ATOM	2203	C44	CHO	L	1	19.179	27.650	18.304	1.00	21.74
ATOM	2204	C48	CHO	L	1	26.193	25.932	18.008	1.00	18.44
ATOM	2205	C50	CHO	L	1	26.277	26.915	16.822	1.00	20.10
ATOM	2206	C54	CHO	L	1	27.502	25.106	18.059	1.00	18.74
ATOM	2207	C57	CHO	L	1	27.623	23.980	17.005	1.00	19.99
ATOM	2208	C60	CHO	L	1	29.075	23.453	17.059	1.00	22.47
ATOM	2209	C63	CHO	L	1	29.308	22.160	16.245	1.00	22.68
ATOM	2210	C65	CHO	L	1	30.827	21.916	16.132	1.00	21.49
ATOM	2211	C69	CHO	L	1	28.658	20.944	16.934	1.00	23.08
ATOM	2212	O73	CHO	L	1	14.905	26.073	16.943	1.00	22.77

END

Table 9

ATOM	1	N	HIS	A	261	-18.369	28.759	-10.025	1.00	60.80	N
ATOM	2	CA	HIS	A	261	-17.481	28.056	-11.002	1.00	61.14	C
ATOM	3	CB	HIS	A	261	-18.304	27.204	-11.961	1.00	61.45	C
ATOM	4	CG	HIS	A	261	-17.529	26.743	-13.153	1.00	63.15	C
ATOM	5	ND1	HIS	A	261	-17.467	27.465	-14.327	1.00	65.59	N
ATOM	6	CE1	HIS	A	261	-16.705	26.824	-15.195	1.00	66.06	C
ATOM	7	NE2	HIS	A	261	-16.255	25.723	-14.620	1.00	66.44	N
ATOM	8	CD2	HIS	A	261	-16.754	25.650	-13.342	1.00	65.64	C
ATOM	9	C	HIS	A	261	-16.640	29.033	-11.812	1.00	60.44	C
ATOM	10	O	HIS	A	261	-15.409	29.012	-11.759	1.00	60.45	O
ATOM	11	N	HIS	A	262	-17.309	29.814	-12.647	1.00	59.75	N
ATOM	12	CA	HIS	A	262	-16.661	30.904	-13.361	1.00	59.30	C
ATOM	13	CB	HIS	A	262	-17.695	31.652	-14.199	1.00	58.98	C
ATOM	14	CG	HIS	A	262	-18.358	30.763	-15.209	1.00	59.57	C
ATOM	15	ND1	HIS	A	262	-19.391	29.908	-14.883	1.00	59.43	N
ATOM	16	CE1	HIS	A	262	-19.744	29.220	-15.954	1.00	60.29	C
ATOM	17	NE2	HIS	A	262	-18.967	29.586	-16.959	1.00	59.72	N
ATOM	18	CD2	HIS	A	262	-18.082	30.538	-16.516	1.00	59.13	C
ATOM	19	C	HIS	A	262	-15.815	31.792	-12.437	1.00	59.09	C
ATOM	20	O	HIS	A	262	-14.698	32.162	-12.810	1.00	58.61	O
ATOM	21	N	LEU	A	263	-16.300	32.109	-11.235	1.00	58.77	N
ATOM	22	CA	LEU	A	263	-15.449	32.829	-10.282	1.00	58.96	C
ATOM	23	CB	LEU	A	263	-16.221	33.286	-9.044	1.00	58.85	C
ATOM	24	CG	LEU	A	263	-16.866	34.666	-9.101	1.00	58.28	C
ATOM	25	CD1	LEU	A	263	-17.642	34.934	-7.824	1.00	57.90	C
ATOM	26	CD2	LEU	A	263	-15.841	35.758	-9.332	1.00	57.75	C
ATOM	27	C	LEU	A	263	-14.261	31.965	-9.840	1.00	59.44	C
ATOM	28	O	LEU	A	263	-13.154	32.463	-9.682	1.00	59.40	O
ATOM	29	N	GLU	A	264	-14.497	30.672	-9.638	1.00	60.29	N
ATOM	30	CA	GLU	A	264	-13.450	29.748	-9.204	1.00	60.91	C
ATOM	31	CB	GLU	A	264	-14.038	28.349	-8.952	1.00	61.72	C
ATOM	32	CG	GLU	A	264	-13.227	27.462	-8.006	1.00	64.54	C
ATOM	33	CD	GLU	A	264	-13.691	25.995	-8.002	1.00	68.63	C
ATOM	34	OE1	GLU	A	264	-14.800	25.693	-7.476	1.00	69.87	O
ATOM	35	OE2	GLU	A	264	-12.934	25.135	-8.534	1.00	70.91	O
ATOM	36	C	GLU	A	264	-12.339	29.694	-10.251	1.00	60.26	C
ATOM	37	O	GLU	A	264	-11.161	29.596	-9.920	1.00	60.38	O
ATOM	38	N	VAL	A	265	-12.709	29.797	-11.516	1.00	59.34	N
ATOM	39	CA	VAL	A	265	-11.722	29.766	-12.574	1.00	58.79	C
ATOM	40	CB	VAL	A	265	-12.393	29.559	-13.923	1.00	58.56	C
ATOM	41	CG1	VAL	A	265	-11.436	29.892	-15.064	1.00	58.68	C
ATOM	42	CG2	VAL	A	265	-12.905	28.140	-14.025	1.00	57.58	C
ATOM	43	C	VAL	A	265	-10.878	31.034	-12.599	1.00	58.95	C
ATOM	44	O	VAL	A	265	-9.689	30.984	-12.896	1.00	58.69	O
ATOM	45	N	LEU	A	266	-11.488	32.164	-12.282	1.00	59.10	N
ATOM	46	CA	LEU	A	266	-10.780	33.433	-12.254	1.00	59.95	C
ATOM	47	CB	LEU	A	266	-11.780	34.586	-12.145	1.00	59.85	C
ATOM	48	CG	LEU	A	266	-12.590	34.829	-13.408	1.00	59.43	C
ATOM	49	CD1	LEU	A	266	-13.498	36.026	-13.226	1.00	58.82	C
ATOM	50	CD2	LEU	A	266	-11.655	35.012	-14.604	1.00	58.96	C
ATOM	51	C	LEU	A	266	-9.777	33.556	-11.108	1.00	60.75	C
ATOM	52	O	LEU	A	266	-8.907	34.423	-11.140	1.00	60.71	O
ATOM	53	N	PHE	A	267	-9.914	32.713	-10.094	1.00	62.00	N
ATOM	54	CA	PHE	A	267	-9.035	32.758	-8.931	1.00	63.40	C
ATOM	55	CB	PHE	A	267	-9.881	32.790	-7.656	1.00	63.54	C
ATOM	56	CG	PHE	A	267	-10.498	34.119	-7.397	1.00	64.83	C
ATOM	57	CD1	PHE	A	267	-11.812	34.368	-7.719	1.00	66.41	C
ATOM	58	CE1	PHE	A	267	-12.367	35.615	-7.500	1.00	67.05	C
ATOM	59	CZ	PHE	A	267	-11.605	36.617	-6.969	1.00	67.09	C
ATOM	60	CE2	PHE	A	267	-10.298	36.382	-6.649	1.00	67.35	C
ATOM	61	CD2	PHE	A	267	-9.745	35.138	-6.864	1.00	66.42	C
ATOM	62	C	PHE	A	267	-8.042	31.595	-8.858	1.00	64.32	C
ATOM	63	O	PHE	A	267	-7.031	31.680	-8.158	1.00	65.16	O
ATOM	64	N	GLN	A	268	-8.325	30.519	-9.587	1.00	64.99	N

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ATOM	65	CA	GLN	A	268	-7.514	29.299	-9.542	1.00	65.36	C
ATOM	66	CB	GLN	A	268	-7.800	28.433	-10.770	1.00	65.80	C
ATOM	67	CG	GLN	A	268	-7.456	26.956	-10.580	1.00	67.88	C
ATOM	68	CD	GLN	A	268	-7.793	26.122	-11.809	1.00	70.56	C
ATOM	69	OE1	GLN	A	268	-8.555	26.568	-12.681	1.00	72.72	O
ATOM	70	NE2	GLN	A	268	-7.223	24.919	-11.891	1.00	71.16	N
ATOM	71	C	GLN	A	268	-6.001	29.518	-9.415	1.00	64.81	C
ATOM	72	O	GLN	A	268	-5.350	28.832	-8.630	1.00	64.77	O
ATOM	73	N	GLY	A	269	-5.441	30.451	-10.180	1.00	64.05	N
ATOM	74	CA	GLY	A	269	-4.005	30.686	-10.129	1.00	63.44	C
ATOM	75	C	GLY	A	269	-3.523	31.020	-8.723	1.00	62.74	C
ATOM	76	O	GLY	A	269	-3.081	30.147	-7.971	1.00	62.53	O
ATOM	77	N	PRO	A	270	-3.623	32.295	-8.369	1.00	61.62	N
ATOM	78	CA	PRO	A	270	-3.226	32.784	-7.046	1.00	60.71	C
ATOM	79	CB	PRO	A	270	-3.788	34.203	-7.019	1.00	61.06	C
ATOM	80	CG	PRO	A	270	-3.818	34.625	-8.460	1.00	61.54	C
ATOM	81	CD	PRO	A	270	-4.122	33.374	-9.238	1.00	61.80	C
ATOM	82	C	PRO	A	270	-3.805	31.980	-5.894	1.00	59.59	C
ATOM	83	O	PRO	A	270	-3.131	31.832	-4.878	1.00	59.46	O
ATOM	84	N	ALA	A	271	-5.019	31.464	-6.034	1.00	57.85	N
ATOM	85	CA	ALA	A	271	-5.583	30.679	-4.955	1.00	56.85	C
ATOM	86	CB	ALA	A	271	-6.933	30.115	-5.330	1.00	56.89	C
ATOM	87	C	ALA	A	271	-4.642	29.553	-4.624	1.00	55.87	C
ATOM	88	O	ALA	A	271	-4.414	29.277	-3.461	1.00	54.85	O
ATOM	89	N	GLU	A	272	-4.123	28.906	-5.669	1.00	55.03	N
ATOM	90	CA	GLU	A	272	-3.219	27.766	-5.542	1.00	54.75	C
ATOM	91	CB	GLU	A	272	-2.898	27.199	-6.926	1.00	55.29	C
ATOM	92	CG	GLU	A	272	-2.191	25.854	-6.930	1.00	58.02	C
ATOM	93	CD	GLU	A	272	-3.117	24.691	-6.580	1.00	62.00	C
ATOM	94	OE1	GLU	A	272	-4.000	24.868	-5.694	1.00	62.47	O
ATOM	95	OE2	GLU	A	272	-2.966	23.598	-7.202	1.00	63.34	O
ATOM	96	C	GLU	A	272	-1.923	28.139	-4.819	1.00	53.60	C
ATOM	97	O	GLU	A	272	-1.420	27.370	-4.019	1.00	52.90	O
ATOM	98	N	LEU	A	273	-1.392	29.323	-5.100	1.00	53.00	N
ATOM	99	CA	LEU	A	273	-0.187	29.775	-4.440	1.00	52.74	C
ATOM	100	CB	LEU	A	273	0.295	31.091	-5.029	1.00	53.24	C
ATOM	101	CG	LEU	A	273	0.578	31.167	-6.522	1.00	54.92	C
ATOM	102	CD1	LEU	A	273	1.291	32.486	-6.819	1.00	55.95	C
ATOM	103	CD2	LEU	A	273	1.400	29.983	-7.007	1.00	56.45	C
ATOM	104	C	LEU	A	273	-0.489	30.012	-2.984	1.00	51.81	C
ATOM	105	O	LEU	A	273	0.302	29.668	-2.103	1.00	51.57	O
ATOM	106	N	GLU	A	274	-1.638	30.629	-2.729	1.00	50.55	N
ATOM	107	CA	GLU	A	274	-2.025	30.937	-1.362	1.00	49.74	C
ATOM	108	CB	GLU	A	274	-3.276	31.827	-1.321	1.00	49.87	C
ATOM	109	CG	GLU	A	274	-3.526	32.505	0.016	1.00	50.96	C
ATOM	110	CD	GLU	A	274	-2.357	33.359	0.481	1.00	52.00	C
ATOM	111	OE1	GLU	A	274	-1.827	34.142	-0.341	1.00	52.15	O
ATOM	112	OE2	GLU	A	274	-1.974	33.236	1.665	1.00	56.29	O
ATOM	113	C	GLU	A	274	-2.248	29.627	-0.629	1.00	48.42	C
ATOM	114	O	GLU	A	274	-1.817	29.475	0.505	1.00	48.21	O
ATOM	115	N	HIS	A	275	-2.879	28.668	-1.285	1.00	47.05	N
ATOM	116	CA	HIS	A	275	-3.148	27.394	-0.623	1.00	46.52	C
ATOM	117	CB	HIS	A	275	-3.928	26.445	-1.530	1.00	46.60	C
ATOM	118	CG	HIS	A	275	-4.241	25.113	-0.905	1.00	48.13	C
ATOM	119	ND1	HIS	A	275	-5.321	24.914	-0.070	1.00	49.08	N
ATOM	120	CE1	HIS	A	275	-5.360	23.647	0.312	1.00	51.04	C
ATOM	121	NE2	HIS	A	275	-4.345	23.009	-0.248	1.00	50.51	N
ATOM	122	CD2	HIS	A	275	-3.631	23.903	-1.019	1.00	50.94	C
ATOM	123	C	HIS	A	275	-1.857	26.721	-0.193	1.00	45.34	C
ATOM	124	O	HIS	A	275	-1.766	26.218	0.917	1.00	45.39	O
ATOM	125	N	LEU	A	276	-0.866	26.692	-1.078	1.00	44.20	N
ATOM	126	CA	LEU	A	276	0.405	26.056	-0.762	1.00	43.43	C
ATOM	127	CB	LEU	A	276	1.243	25.889	-2.034	1.00	43.73	C
ATOM	128	CG	LEU	A	276	2.652	25.291	-1.877	1.00	43.56	C
ATOM	129	CD1	LEU	A	276	2.568	23.818	-1.557	1.00	43.50	C
ATOM	130	CD2	LEU	A	276	3.486	25.536	-3.127	1.00	43.26	C

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ATOM	131	C	LEU	A	276	1.172	26.881	0.310	1.00	42.47	C
ATOM	132	O	LEU	A	276	1.879	26.346	1.153	1.00	40.97	O
ATOM	133	N	ALA	A	277	1.035	28.190	0.302	1.00	41.76	N
ATOM	134	CA	ALA	A	277	1.737	28.961	1.324	1.00	41.55	CA
ATOM	135	CB	ALA	A	277	1.716	30.419	1.004	1.00	41.80	CB
ATOM	136	C	ALA	A	277	1.124	28.718	2.699	1.00	41.51	C
ATOM	137	O	ALA	A	277	1.832	28.631	3.708	1.00	41.21	O
ATOM	138	N	GLN	A	278	-0.192	28.545	2.734	1.00	41.43	N
ATOM	139	CA	GLN	A	278	-0.870	28.331	4.000	1.00	41.87	CA
ATOM	140	CB	GLN	A	278	-2.373	28.610	3.879	1.00	42.96	CB
ATOM	141	CG	GLN	A	278	-2.684	30.122	3.749	1.00	45.63	CG
ATOM	142	CD	GLN	A	278	-4.182	30.476	3.501	1.00	49.42	CD
ATOM	143	OE1	GLN	A	278	-5.098	29.751	3.921	1.00	52.18	OE1
ATOM	144	NE2	GLN	A	278	-4.410	31.605	2.836	1.00	50.77	NE2
ATOM	145	C	GLN	A	278	-0.570	26.945	4.521	1.00	40.99	C
ATOM	146	O	GLN	A	278	-0.411	26.736	5.719	1.00	40.26	O
ATOM	147	N	ASN	A	279	-0.449	25.993	3.621	1.00	40.42	N
ATOM	148	CA	ASN	A	279	-0.117	24.635	4.021	1.00	40.51	CA
ATOM	149	CB	ASN	A	279	-0.075	23.755	2.795	1.00	41.05	CB
ATOM	150	CG	ASN	A	279	0.276	22.322	3.120	1.00	44.76	CG
ATOM	151	OD1	ASN	A	279	-0.554	21.573	3.640	1.00	48.82	OD1
ATOM	152	ND2	ASN	A	279	1.522	21.922	2.818	1.00	51.37	ND2
ATOM	153	C	ASN	A	279	1.242	24.550	4.702	1.00	39.60	C
ATOM	154	O	ASN	A	279	1.411	23.920	5.746	1.00	40.22	O
ATOM	155	N	ILE	A	280	2.219	25.170	4.073	1.00	38.39	N
ATOM	156	CA	ILE	A	280	3.563	25.150	4.550	1.00	37.67	CA
ATOM	157	CB	ILE	A	280	4.493	25.612	3.419	1.00	37.61	CB
ATOM	158	CG1	ILE	A	280	4.506	24.532	2.322	1.00	38.20	CG1
ATOM	159	CD1	ILE	A	280	5.666	24.586	1.341	1.00	39.82	CD1
ATOM	160	CG2	ILE	A	280	5.892	25.864	3.974	1.00	38.20	CG2
ATOM	161	C	ILE	A	280	3.697	25.986	5.823	1.00	36.72	C
ATOM	162	O	ILE	A	280	4.355	25.583	6.765	1.00	35.34	O
ATOM	163	N	SER	A	281	3.060	27.146	5.842	1.00	36.72	N
ATOM	164	CA	SER	A	281	3.018	27.979	7.043	1.00	36.93	CA
ATOM	165	CB	SER	A	281	2.091	29.161	6.831	1.00	37.23	CB
ATOM	166	OG	SER	A	281	2.681	30.069	5.909	1.00	38.94	OG
ATOM	167	C	SER	A	281	2.543	27.219	8.237	1.00	36.20	C
ATOM	168	O	SER	A	281	3.131	27.298	9.295	1.00	35.96	O
ATOM	169	N	LYS	A	282	1.467	26.470	8.068	1.00	36.67	N
ATOM	170	CA	LYS	A	282	0.880	25.704	9.158	1.00	37.15	CA
ATOM	171	CB	LYS	A	282	-0.479	25.107	8.730	1.00	38.10	CB
ATOM	172	CG	LYS	A	282	-1.305	24.498	9.860	1.00	40.15	CG
ATOM	173	CD	LYS	A	282	-2.704	24.142	9.337	1.00	46.19	CD
ATOM	174	CE	LYS	A	282	-3.414	23.021	10.139	1.00	49.27	CE
ATOM	175	NZ	LYS	A	282	-3.455	21.732	9.376	1.00	51.98	NZ
ATOM	176	C	LYS	A	282	1.794	24.585	9.604	1.00	36.50	C
ATOM	177	O	LYS	A	282	1.940	24.307	10.798	1.00	35.79	O
ATOM	178	N	SER	A	283	2.409	23.916	8.643	1.00	35.63	N
ATOM	179	CA	SER	A	283	3.316	22.836	8.997	1.00	34.48	CA
ATOM	180	CB	SER	A	283	3.848	22.181	7.744	1.00	34.45	CB
ATOM	181	OG	SER	A	283	2.754	21.707	7.003	1.00	34.06	OG
ATOM	182	C	SER	A	283	4.441	23.381	9.830	1.00	33.76	C
ATOM	183	O	SER	A	283	4.830	22.758	10.789	1.00	33.46	O
ATOM	184	N	HIS	A	284	4.943	24.552	9.471	1.00	33.35	N
ATOM	185	CA	HIS	A	284	6.007	25.195	10.224	1.00	34.42	CA
ATOM	186	CB	HIS	A	284	6.402	26.460	9.513	1.00	34.00	CB
ATOM	187	CG	HIS	A	284	7.306	27.355	10.288	1.00	34.20	CG
ATOM	188	ND1	HIS	A	284	8.677	27.240	10.249	1.00	32.90	ND1
ATOM	189	CE1	HIS	A	284	9.221	28.201	10.968	1.00	33.90	CE1
ATOM	190	NE2	HIS	A	284	8.249	28.946	11.472	1.00	35.01	NE2
ATOM	191	CD2	HIS	A	284	7.042	28.448	11.045	1.00	36.29	CD2
ATOM	192	C	HIS	A	284	5.629	25.530	11.660	1.00	35.30	C
ATOM	193	O	HIS	A	284	6.391	25.244	12.589	1.00	34.75	O
ATOM	194	N	LEU	A	285	4.469	26.172	11.824	1.00	36.71	N
ATOM	195	CA	LEU	A	285	3.947	26.548	13.136	1.00	37.40	CA
ATOM	196	CB	LEU	A	285	2.579	27.208	12.997	1.00	38.70	CB

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ATOM	197	CG	LEU	A	285	1.838	27.637	14.272	1.00	41.84	C
ATOM	198	CD1	LEU	A	285	2.525	28.826	14.913	1.00	42.97	C
ATOM	199	CD2	LEU	A	285	0.385	27.982	13.934	1.00	43.37	C
ATOM	200	C	LEU	A	285	3.846	25.351	14.046	1.00	37.27	C
ATOM	201	O	LEU	A	285	4.279	25.403	15.206	1.00	37.97	O
ATOM	202	N	GLU	A	286	3.369	24.237	13.510	1.00	36.60	N
ATOM	203	CA	GLU	A	286	3.134	23.058	14.337	1.00	36.96	C
ATOM	204	CB	GLU	A	286	1.988	22.229	13.722	1.00	37.46	C
ATOM	205	CG	GLU	A	286	0.751	23.091	13.462	1.00	42.20	C
ATOM	206	CD	GLU	A	286	-0.487	22.289	13.142	1.00	48.25	C
ATOM	207	OE1	GLU	A	286	-0.343	21.219	12.510	1.00	52.12	O
ATOM	208	OE2	GLU	A	286	-1.601	22.726	13.534	1.00	52.12	O
ATOM	209	C	GLU	A	286	4.350	22.157	14.572	1.00	35.80	C
ATOM	210	O	GLU	A	286	4.231	21.190	15.303	1.00	34.55	O
ATOM	211	N	THR	A	287	5.485	22.439	13.931	1.00	34.46	N
ATOM	212	CA	THR	A	287	6.684	21.616	14.118	1.00	34.18	C
ATOM	213	CB	THR	A	287	7.154	20.957	12.814	1.00	33.50	C
ATOM	214	OG1	THR	A	287	7.367	21.952	11.807	1.00	30.59	O
ATOM	215	CG2	THR	A	287	6.122	20.050	12.250	1.00	34.40	C
ATOM	216	C	THR	A	287	7.879	22.382	14.670	1.00	34.80	C
ATOM	217	O	THR	A	287	8.965	21.849	14.681	1.00	35.10	O
ATOM	218	N	CYS	A	288	7.709	23.638	15.047	1.00	35.78	N
ATOM	219	CA	CYS	A	288	8.764	24.346	15.740	1.00	36.72	C
ATOM	220	CB	CYS	A	288	8.642	25.851	15.552	1.00	36.32	C
ATOM	221	SG	CYS	A	288	9.235	26.481	13.966	1.00	39.84	S
ATOM	222	C	CYS	A	288	8.682	23.996	17.230	1.00	36.71	C
ATOM	223	O	CYS	A	288	7.602	23.895	17.792	1.00	36.87	O
ATOM	224	N	GLN	A	289	9.830	23.812	17.866	1.00	37.19	N
ATOM	225	CA	GLN	A	289	9.862	23.516	19.278	1.00	37.25	C
ATOM	226	CB	GLN	A	289	11.279	23.153	19.694	1.00	37.24	C
ATOM	227	CG	GLN	A	289	11.409	22.864	21.168	1.00	38.95	C
ATOM	228	CD	GLN	A	289	12.661	22.072	21.551	1.00	40.39	C
ATOM	229	OE1	GLN	A	289	13.694	22.091	20.847	1.00	39.04	O
ATOM	230	NE2	GLN	A	289	12.567	21.369	22.682	1.00	38.81	N
ATOM	231	C	GLN	A	289	9.288	24.683	20.141	1.00	37.72	C
ATOM	232	O	GLN	A	289	8.603	24.432	21.124	1.00	37.80	O
ATOM	233	N	TYR	A	290	9.519	25.935	19.744	1.00	38.28	N
ATOM	234	CA	TYR	A	290	9.072	27.105	20.501	1.00	38.43	C
ATOM	235	CB	TYR	A	290	10.268	27.813	21.152	1.00	38.66	C
ATOM	236	CG	TYR	A	290	11.241	26.912	21.906	1.00	37.22	C
ATOM	237	CD1	TYR	A	290	12.438	26.540	21.332	1.00	35.94	C
ATOM	238	CE1	TYR	A	290	13.339	25.731	21.989	1.00	34.88	C
ATOM	239	CZ	TYR	A	290	13.061	25.293	23.244	1.00	35.86	C
ATOM	240	OH	TYR	A	290	13.983	24.491	23.870	1.00	34.34	O
ATOM	241	CE2	TYR	A	290	11.872	25.660	23.866	1.00	36.55	C
ATOM	242	CD2	TYR	A	290	10.978	26.487	23.193	1.00	35.75	C
ATOM	243	C	TYR	A	290	8.329	28.158	19.650	1.00	39.65	C
ATOM	244	O	TYR	A	290	8.582	28.309	18.443	1.00	39.27	O
ATOM	245	N	LEU	A	291	7.443	28.924	20.296	1.00	40.18	N
ATOM	246	CA	LEU	A	291	6.740	29.985	19.611	1.00	40.92	C
ATOM	247	CB	LEU	A	291	5.444	30.367	20.327	1.00	41.69	C
ATOM	248	CG	LEU	A	291	4.371	29.301	20.591	1.00	43.47	C
ATOM	249	CD1	LEU	A	291	3.295	29.850	21.586	1.00	45.13	C
ATOM	250	CD2	LEU	A	291	3.716	28.890	19.300	1.00	43.40	C
ATOM	251	C	LEU	A	291	7.635	31.202	19.487	1.00	41.12	C
ATOM	252	O	LEU	A	291	8.382	31.554	20.393	1.00	40.66	O
ATOM	253	N	ARG	A	292	7.508	31.876	18.356	1.00	41.62	N
ATOM	254	CA	ARG	A	292	8.317	33.034	18.065	1.00	42.34	C
ATOM	255	CB	ARG	A	292	7.830	33.695	16.766	1.00	42.90	C
ATOM	256	CG	ARG	A	292	8.712	34.814	16.241	1.00	45.07	C
ATOM	257	CD	ARG	A	292	10.053	34.331	15.752	1.00	48.94	C
ATOM	258	NE	ARG	A	292	10.873	35.373	15.134	1.00	50.47	N
ATOM	259	CZ	ARG	A	292	10.786	35.746	13.871	1.00	54.17	C
ATOM	260	NH1	ARG	A	292	9.874	35.206	13.051	1.00	55.75	N
ATOM	261	NH2	ARG	A	292	11.605	36.684	13.420	1.00	55.53	N
ATOM	262	C	ARG	A	292	8.206	34.005	19.199	1.00	42.41	C

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ATOM	263	O	ARG	A	292	9.213	34.496	19.732	1.00	41.10	O
ATOM	264	N	GLU	A	293	6.958	34.287	19.564	1.00	43.20	N
ATOM	265	CA	GLU	A	293	6.675	35.284	20.586	1.00	43.83	C
ATOM	266	CB	GLU	A	293	5.164	35.519	20.679	1.00	44.63	C
ATOM	267	CG	GLU	A	293	4.562	36.144	19.410	1.00	47.94	C
ATOM	268	CD	GLU	A	293	4.517	35.201	18.194	1.00	51.44	C
ATOM	269	OE1	GLU	A	293	4.477	33.955	18.392	1.00	52.38	O
ATOM	270	OE2	GLU	A	293	4.516	35.711	17.033	1.00	52.22	O
ATOM	271	C	GLU	A	293	7.299	34.887	21.928	1.00	43.00	C
ATOM	272	O	GLU	A	293	7.878	35.732	22.598	1.00	43.39	O
ATOM	273	N	GLU	A	294	7.207	33.613	22.303	1.00	42.66	N
ATOM	274	CA	GLU	A	294	7.870	33.111	23.522	1.00	42.27	C
ATOM	275	CB	GLU	A	294	7.845	31.564	23.632	1.00	43.09	C
ATOM	276	CG	GLU	A	294	6.544	30.813	23.909	1.00	45.45	C
ATOM	277	CD	GLU	A	294	6.529	29.398	23.262	1.00	47.89	C
ATOM	278	OE1	GLU	A	294	7.355	28.479	23.591	1.00	42.98	O
ATOM	279	OE2	GLU	A	294	5.666	29.204	22.369	1.00	50.76	O
ATOM	280	C	GLU	A	294	9.364	33.469	23.488	1.00	40.96	C
ATOM	281	O	GLU	A	294	9.919	33.993	24.447	1.00	40.53	O
ATOM	282	N	LEU	A	295	10.017	33.106	22.388	1.00	39.12	N
ATOM	283	CA	LEU	A	295	11.462	33.297	22.239	1.00	38.55	C
ATOM	284	CB	LEU	A	295	11.959	32.681	20.918	1.00	38.19	C
ATOM	285	CG	LEU	A	295	11.815	31.163	20.806	1.00	38.68	C
ATOM	286	CD1	LEU	A	295	11.654	30.733	19.372	1.00	40.29	C
ATOM	287	CD2	LEU	A	295	13.003	30.450	21.445	1.00	38.56	C
ATOM	288	C	LEU	A	295	11.866	34.759	22.318	1.00	37.73	C
ATOM	289	O	LEU	A	295	12.884	35.075	22.907	1.00	36.93	O
ATOM	290	N	GLN	A	296	11.052	35.640	21.749	1.00	38.09	N
ATOM	291	CA	GLN	A	296	11.323	37.083	21.755	1.00	39.08	C
ATOM	292	CB	GLN	A	296	10.390	37.802	20.775	1.00	39.49	C
ATOM	293	CG	GLN	A	296	10.709	37.498	19.284	1.00	43.93	C
ATOM	294	CD	GLN	A	296	9.671	38.037	18.263	1.00	47.60	C
ATOM	295	OE1	GLN	A	296	8.471	38.104	18.537	1.00	50.71	O
ATOM	296	NE2	GLN	A	296	10.152	38.397	17.079	1.00	49.60	N
ATOM	297	C	GLN	A	296	11.203	37.728	23.148	1.00	38.56	C
ATOM	298	O	GLN	A	296	11.898	38.696	23.461	1.00	38.91	O
ATOM	299	N	GLN	A	297	10.351	37.176	23.988	1.00	38.53	N
ATOM	300	CA	GLN	A	297	10.104	37.771	25.297	1.00	38.64	C
ATOM	301	CB	GLN	A	297	8.692	37.402	25.783	1.00	38.82	C
ATOM	302	CG	GLN	A	297	7.621	38.365	25.195	1.00	42.59	C
ATOM	303	CD	GLN	A	297	6.170	37.850	25.288	1.00	48.07	C
ATOM	304	OE1	GLN	A	297	5.797	37.151	26.239	1.00	50.31	O
ATOM	305	NE2	GLN	A	297	5.356	38.199	24.289	1.00	51.73	N
ATOM	306	C	GLN	A	297	11.177	37.428	26.347	1.00	37.73	C
ATOM	307	O	GLN	A	297	11.210	38.040	27.413	1.00	37.76	O
ATOM	308	N	ILE	A	298	12.045	36.452	26.059	1.00	36.25	N
ATOM	309	CA	ILE	A	298	13.087	36.084	27.007	1.00	34.28	C
ATOM	310	CB	ILE	A	298	12.920	34.651	27.472	1.00	34.23	C
ATOM	311	CG1	ILE	A	298	12.999	33.705	26.282	1.00	34.17	C
ATOM	312	CD1	ILE	A	298	13.013	32.277	26.693	1.00	37.43	C
ATOM	313	CG2	ILE	A	298	11.588	34.413	28.205	1.00	36.82	C
ATOM	314	C	ILE	A	298	14.520	36.278	26.479	1.00	32.82	C
ATOM	315	O	ILE	A	298	15.421	35.612	26.959	1.00	32.45	O
ATOM	316	N	THR	A	299	14.748	37.175	25.518	1.00	32.29	N
ATOM	317	CA	THR	A	299	16.110	37.434	25.027	1.00	32.00	C
ATOM	318	CB	THR	A	299	16.149	38.398	23.832	1.00	32.50	C
ATOM	319	OG1	THR	A	299	15.244	39.478	24.047	1.00	34.44	O
ATOM	320	CG2	THR	A	299	15.653	37.762	22.528	1.00	33.01	C
ATOM	321	C	THR	A	299	17.000	38.007	26.104	1.00	31.05	C
ATOM	322	O	THR	A	299	18.212	37.917	26.015	1.00	30.68	O
ATOM	323	N	TRP	A	300	16.412	38.607	27.132	1.00	30.79	N
ATOM	324	CA	TRP	A	300	17.218	39.162	28.237	1.00	29.80	C
ATOM	325	CB	TRP	A	300	16.413	40.155	29.094	1.00	29.57	C
ATOM	326	CG	TRP	A	300	15.189	39.547	29.664	1.00	27.22	C
ATOM	327	CD1	TRP	A	300	13.988	39.423	29.044	1.00	25.70	C
ATOM	328	NE1	TRP	A	300	13.096	38.775	29.862	1.00	24.08	N

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ATOM	329	CE2	TRP	A	300	13.727	38.462	31.033	1.00	24.93	C
ATOM	330	CD2	TRP	A	300	15.045	38.926	30.936	1.00	23.62	C
ATOM	331	CE3	TRP	A	300	15.884	38.761	32.030	1.00	26.31	C
ATOM	332	CZ3	TRP	A	300	15.415	38.153	33.128	1.00	27.39	C
ATOM	333	CH2	TRP	A	300	14.083	37.700	33.201	1.00	28.78	C
ATOM	334	CZ2	TRP	A	300	13.231	37.857	32.168	1.00	24.74	C
ATOM	335	C	TRP	A	300	17.803	38.099	29.155	1.00	29.45	C
ATOM	336	O	TRP	A	300	18.751	38.365	29.906	1.00	30.38	O
ATOM	337	N	GLN	A	301	17.231	36.897	29.103	1.00	29.27	N
ATOM	338	CA	GLN	A	301	17.695	35.781	29.923	1.00	29.27	C
ATOM	339	CB	GLN	A	301	16.616	34.701	30.038	1.00	28.84	C
ATOM	340	CG	GLN	A	301	15.419	35.171	30.791	1.00	30.22	C
ATOM	341	CD	GLN	A	301	14.251	34.170	30.897	1.00	33.05	C
ATOM	342	OE1	GLN	A	301	14.340	33.032	30.464	1.00	32.79	O
ATOM	343	NE2	GLN	A	301	13.144	34.633	31.479	1.00	34.45	N
ATOM	344	C	GLN	A	301	18.964	35.186	29.327	1.00	29.50	C
ATOM	345	O	GLN	A	301	18.926	34.117	28.725	1.00	30.22	O
ATOM	346	N	THR	A	302	20.081	35.884	29.484	1.00	29.33	N
ATOM	347	CA	THR	A	302	21.372	35.407	29.007	1.00	29.03	C
ATOM	348	CB	THR	A	302	22.271	36.588	28.567	1.00	29.13	C
ATOM	349	OG1	THR	A	302	22.307	37.572	29.603	1.00	28.27	O
ATOM	350	CG2	THR	A	302	21.695	37.317	27.362	1.00	29.18	C
ATOM	351	C	THR	A	302	22.024	34.662	30.165	1.00	29.23	C
ATOM	352	O	THR	A	302	21.615	34.836	31.308	1.00	29.31	O
ATOM	353	N	PHE	A	303	22.987	33.791	29.874	1.00	29.05	N
ATOM	354	CA	PHE	A	303	23.704	33.101	30.929	1.00	29.57	C
ATOM	355	CB	PHE	A	303	24.678	32.033	30.380	1.00	29.12	C
ATOM	356	CG	PHE	A	303	23.998	30.815	29.837	1.00	27.07	C
ATOM	357	CD1	PHE	A	303	23.798	30.691	28.475	1.00	27.05	C
ATOM	358	CE1	PHE	A	303	23.156	29.630	27.957	1.00	27.11	C
ATOM	359	CZ	PHE	A	303	22.699	28.639	28.795	1.00	27.76	C
ATOM	360	CE2	PHE	A	303	22.884	28.746	30.156	1.00	27.13	C
ATOM	361	CD2	PHE	A	303	23.530	29.833	30.669	1.00	26.38	C
ATOM	362	C	PHE	A	303	24.461	34.134	31.780	1.00	30.22	C
ATOM	363	O	PHE	A	303	24.913	35.153	31.291	1.00	30.40	O
ATOM	364	N	LEU	A	304	24.598	33.854	33.053	1.00	31.25	N
ATOM	365	CA	LEU	A	304	25.332	34.733	33.954	1.00	32.65	C
ATOM	366	CB	LEU	A	304	24.930	34.475	35.390	1.00	32.80	C
ATOM	367	CG	LEU	A	304	23.457	34.647	35.722	1.00	33.60	C
ATOM	368	CD1	LEU	A	304	23.213	34.101	37.076	1.00	35.11	C
ATOM	369	CD2	LEU	A	304	23.051	36.084	35.695	1.00	35.33	C
ATOM	370	C	LEU	A	304	26.800	34.424	33.797	1.00	34.30	C
ATOM	371	O	LEU	A	304	27.171	33.345	33.332	1.00	32.86	O
ATOM	372	N	GLN	A	305	27.647	35.360	34.195	1.00	36.15	N
ATOM	373	CA	GLN	A	305	29.077	35.180	34.006	1.00	38.54	C
ATOM	374	CB	GLN	A	305	29.852	36.381	34.584	1.00	39.68	C
ATOM	375	CG	GLN	A	305	31.293	36.596	34.029	1.00	42.48	C
ATOM	376	CD	GLN	A	305	31.436	36.533	32.488	1.00	46.39	C
ATOM	377	OE1	GLN	A	305	30.636	37.118	31.720	1.00	46.08	O
ATOM	378	NE2	GLN	A	305	32.497	35.850	32.041	1.00	48.27	N
ATOM	379	C	GLN	A	305	29.584	33.832	34.575	1.00	38.86	C
ATOM	380	O	GLN	A	305	30.428	33.194	33.968	1.00	39.34	O
ATOM	381	N	GLU	A	306	29.031	33.391	35.698	1.00	39.71	N
ATOM	382	CA	GLU	A	306	29.451	32.155	36.350	1.00	39.99	C
ATOM	383	CB	GLU	A	306	28.756	31.992	37.705	1.00	41.15	C
ATOM	384	CG	GLU	A	306	29.089	33.078	38.735	1.00	47.39	C
ATOM	385	CD	GLU	A	306	28.167	33.080	39.980	1.00	55.43	C
ATOM	386	OE1	GLU	A	306	27.643	31.999	40.357	1.00	59.46	O
ATOM	387	OE2	GLU	A	306	27.962	34.167	40.612	1.00	60.68	O
ATOM	388	C	GLU	A	306	29.132	30.952	35.472	1.00	38.37	C
ATOM	389	O	GLU	A	306	29.926	30.022	35.353	1.00	38.01	O
ATOM	390	N	GLU	A	307	27.943	30.967	34.889	1.00	36.34	N
ATOM	391	CA	GLU	A	307	27.514	29.927	33.988	1.00	34.63	C
ATOM	392	CB	GLU	A	307	26.032	30.117	33.642	1.00	35.14	C
ATOM	393	CG	GLU	A	307	25.062	30.047	34.823	1.00	34.93	C
ATOM	394	CD	GLU	A	307	23.620	30.319	34.412	1.00	36.18	C

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ATOM	395	OE1	GLU	A	307	22.785	29.382	34.543	1.00	36.82	O
ATOM	396	OE2	GLU	A	307	23.312	31.467	33.946	1.00	32.29	O
ATOM	397	C	GLU	A	307	28.395	29.957	32.716	1.00	33.42	C
ATOM	398	O	GLU	A	307	28.752	28.907	32.177	1.00	30.28	O
ATOM	399	N	ILE	A	308	28.778	31.149	32.264	1.00	32.73	N
ATOM	400	CA	ILE	A	308	29.593	31.251	31.062	1.00	33.52	C
ATOM	401	CB	ILE	A	308	29.723	32.701	30.595	1.00	33.62	C
ATOM	402	CG1	ILE	A	308	28.384	33.198	30.061	1.00	34.47	C
ATOM	403	CD1	ILE	A	308	28.385	34.618	29.697	1.00	34.55	C
ATOM	404	CG2	ILE	A	308	30.758	32.864	29.484	1.00	33.46	C
ATOM	405	C	ILE	A	308	30.933	30.564	31.324	1.00	34.15	C
ATOM	406	O	ILE	A	308	31.373	29.709	30.560	1.00	33.82	O
ATOM	407	N	GLU	A	309	31.549	30.899	32.447	1.00	35.66	N
ATOM	408	CA	GLU	A	309	32.813	30.284	32.858	1.00	36.34	C
ATOM	409	CB	GLU	A	309	33.280	30.879	34.199	1.00	37.37	C
ATOM	410	CG	GLU	A	309	33.860	32.290	34.048	1.00	41.64	C
ATOM	411	CD	GLU	A	309	33.687	33.171	35.295	1.00	46.42	C
ATOM	412	OE1	GLU	A	309	33.419	32.615	36.387	1.00	49.14	O
ATOM	413	OE2	GLU	A	309	33.805	34.426	35.174	1.00	51.22	O
ATOM	414	C	GLU	A	309	32.718	28.766	32.941	1.00	35.17	C
ATOM	415	O	GLU	A	309	33.580	28.072	32.431	1.00	35.55	O
ATOM	416	N	ASN	A	310	31.679	28.249	33.578	1.00	34.21	N
ATOM	417	CA	ASN	A	310	31.478	26.817	33.603	1.00	34.07	C
ATOM	418	CB	ASN	A	310	30.168	26.511	34.282	1.00	35.39	C
ATOM	419	CG	ASN	A	310	29.871	25.036	34.346	1.00	38.20	C
ATOM	420	OD1	ASN	A	310	30.608	24.260	34.994	1.00	45.99	O
ATOM	421	ND2	ASN	A	310	28.778	24.629	33.712	1.00	42.62	N
ATOM	422	C	ASN	A	310	31.488	26.202	32.212	1.00	33.34	C
ATOM	423	O	ASN	A	310	32.171	25.193	31.987	1.00	33.73	O
ATOM	424	N	TYR	A	311	30.780	26.795	31.247	1.00	31.41	N
ATOM	425	CA	TYR	A	311	30.793	26.215	29.919	1.00	30.92	C
ATOM	426	CB	TYR	A	311	29.821	26.904	28.959	1.00	30.60	C
ATOM	427	CG	TYR	A	311	28.362	26.519	29.117	1.00	29.73	C
ATOM	428	CD1	TYR	A	311	27.421	27.465	29.445	1.00	28.73	C
ATOM	429	CE1	TYR	A	311	26.090	27.149	29.590	1.00	29.50	C
ATOM	430	CZ	TYR	A	311	25.671	25.875	29.403	1.00	29.74	C
ATOM	431	OH	TYR	A	311	24.332	25.610	29.557	1.00	32.23	O
ATOM	432	CE2	TYR	A	311	26.578	24.897	29.056	1.00	29.37	C
ATOM	433	CD2	TYR	A	311	27.925	25.224	28.915	1.00	29.13	C
ATOM	434	C	TYR	A	311	32.192	26.310	29.367	1.00	31.46	C
ATOM	435	O	TYR	A	311	32.635	25.434	28.636	1.00	30.86	O
ATOM	436	N	GLN	A	312	32.890	27.398	29.688	1.00	32.56	N
ATOM	437	CA	GLN	A	312	34.251	27.554	29.209	1.00	33.54	C
ATOM	438	CB	GLN	A	312	34.706	29.010	29.300	1.00	33.50	C
ATOM	439	CG	GLN	A	312	34.082	29.859	28.239	1.00	33.49	C
ATOM	440	CD	GLN	A	312	34.392	31.302	28.461	1.00	34.18	C
ATOM	441	OE1	GLN	A	312	34.841	31.667	29.542	1.00	35.47	O
ATOM	442	NE2	GLN	A	312	34.172	32.127	27.449	1.00	31.68	N
ATOM	443	C	GLN	A	312	35.202	26.603	29.928	1.00	34.41	C
ATOM	444	O	GLN	A	312	36.250	26.270	29.394	1.00	34.43	O
ATOM	445	N	ASN	A	313	34.834	26.151	31.116	1.00	35.17	N
ATOM	446	CA	ASN	A	313	35.680	25.192	31.827	1.00	36.70	C
ATOM	447	CB	ASN	A	313	35.383	25.209	33.333	1.00	37.66	C
ATOM	448	CG	ASN	A	313	35.992	26.423	34.051	1.00	41.22	C
ATOM	449	OD1	ASN	A	313	36.882	27.096	33.522	1.00	42.54	O
ATOM	450	ND2	ASN	A	313	35.478	26.717	35.265	1.00	44.69	N
ATOM	451	C	ASN	A	313	35.531	23.745	31.310	1.00	36.84	C
ATOM	452	O	ASN	A	313	36.405	22.889	31.568	1.00	36.22	O
ATOM	453	N	LYS	A	314	34.412	23.459	30.619	1.00	36.29	N
ATOM	454	CA	LYS	A	314	34.166	22.111	30.110	1.00	35.35	C
ATOM	455	CB	LYS	A	314	32.761	21.940	29.527	1.00	35.14	C
ATOM	456	CG	LYS	A	314	31.628	22.032	30.526	1.00	35.45	C
ATOM	457	CD	LYS	A	314	30.290	21.978	29.787	1.00	38.14	C
ATOM	458	CE	LYS	A	314	29.085	22.009	30.733	1.00	39.70	C
ATOM	459	NZ	LYS	A	314	29.206	21.049	31.917	1.00	44.38	N
ATOM	460	C	LYS	A	314	35.186	21.752	29.052	1.00	35.29	C



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ATOM	461	O	LYS	A	314	35.676	22.605	28.307	1.00	35.12	O
ATOM	462	N	GLN	A	315	35.484	20.452	29.000	1.00	34.85	N
ATOM	463	CA	GLN	A	315	36.430	19.906	28.048	1.00	34.64	C
ATOM	464	CB	GLN	A	315	36.771	18.469	28.417	1.00	34.90	C
ATOM	465	CG	GLN	A	315	37.502	18.260	29.733	1.00	39.29	C
ATOM	466	CD	GLN	A	315	38.919	18.804	29.697	1.00	44.94	C
ATOM	467	OE1	GLN	A	315	39.685	18.490	28.787	1.00	50.63	O
ATOM	468	NE2	GLN	A	315	39.264	19.634	30.677	1.00	47.61	N
ATOM	469	C	GLN	A	315	35.846	19.884	26.647	1.00	33.86	C
ATOM	470	O	GLN	A	315	34.631	19.748	26.460	1.00	32.99	O
ATOM	471	N	ARG	A	316	36.729	19.965	25.664	1.00	32.95	N
ATOM	472	CA	ARG	A	316	36.315	19.977	24.292	1.00	32.86	C
ATOM	473	CB	ARG	A	316	37.519	19.829	23.385	1.00	33.76	C
ATOM	474	CG	ARG	A	316	37.205	20.195	21.947	1.00	38.32	C
ATOM	475	CD	ARG	A	316	38.414	20.275	21.047	1.00	43.87	C
ATOM	476	NE	ARG	A	316	38.022	20.301	19.640	1.00	49.79	N
ATOM	477	CZ	ARG	A	316	38.804	19.922	18.624	1.00	53.81	C
ATOM	478	NH1	ARG	A	316	40.036	19.479	18.847	1.00	55.22	N
ATOM	479	NH2	ARG	A	316	38.347	19.990	17.381	1.00	55.07	N
ATOM	480	C	ARG	A	316	35.289	18.895	23.966	1.00	31.22	C
ATOM	481	O	ARG	A	316	34.241	19.187	23.405	1.00	28.96	O
ATOM	482	N	GLU	A	317	35.575	17.649	24.327	1.00	30.76	N
ATOM	483	CA	GLU	A	317	34.680	16.574	23.930	1.00	30.63	C
ATOM	484	CB	GLU	A	317	35.315	15.181	24.082	1.00	31.32	C
ATOM	485	CG	GLU	A	317	35.547	14.697	25.484	1.00	33.23	C
ATOM	486	CD	GLU	A	317	36.850	15.194	26.090	1.00	38.72	C
ATOM	487	OE1	GLU	A	317	37.349	14.502	27.024	1.00	44.77	O
ATOM	488	OE2	GLU	A	317	37.365	16.259	25.674	1.00	34.98	O
ATOM	489	C	GLU	A	317	33.351	16.695	24.640	1.00	29.33	C
ATOM	490	O	GLU	A	317	32.344	16.314	24.099	1.00	30.11	O
ATOM	491	N	VAL	A	318	33.365	17.256	25.829	1.00	27.92	N
ATOM	492	CA	VAL	A	318	32.173	17.464	26.628	1.00	27.86	C
ATOM	493	CB	VAL	A	318	32.529	17.835	28.082	1.00	28.20	C
ATOM	494	CG1	VAL	A	318	31.275	18.177	28.870	1.00	28.77	C
ATOM	495	CG2	VAL	A	318	33.263	16.646	28.741	1.00	29.97	C
ATOM	496	C	VAL	A	318	31.244	18.528	26.013	1.00	27.21	C
ATOM	497	O	VAL	A	318	30.048	18.287	25.886	1.00	26.50	O
ATOM	498	N	MET	A	319	31.799	19.670	25.603	1.00	26.29	N
ATOM	499	CA	MET	A	319	31.018	20.716	24.961	1.00	26.24	C
ATOM	500	CB	MET	A	319	31.852	22.004	24.831	1.00	27.30	C
ATOM	501	CG	MET	A	319	31.050	23.268	24.597	1.00	28.90	C
ATOM	502	SD	MET	A	319	29.794	23.654	25.828	1.00	33.36	S
ATOM	503	CE	MET	A	319	28.848	24.807	24.932	1.00	31.15	C
ATOM	504	C	MET	A	319	30.472	20.228	23.615	1.00	25.53	C
ATOM	505	O	MET	A	319	29.325	20.447	23.281	1.00	25.99	O
ATOM	506	N	TRP	A	320	31.267	19.511	22.857	1.00	25.05	N
ATOM	507	CA	TRP	A	320	30.790	18.939	21.621	1.00	24.82	C
ATOM	508	CB	TRP	A	320	31.923	18.183	20.921	1.00	24.80	C
ATOM	509	CG	TRP	A	320	32.634	18.949	19.867	1.00	27.31	C
ATOM	510	CD1	TRP	A	320	33.705	19.786	20.039	1.00	30.43	C
ATOM	511	NE1	TRP	A	320	34.100	20.301	18.831	1.00	31.02	N
ATOM	512	CE2	TRP	A	320	33.268	19.826	17.854	1.00	28.25	C
ATOM	513	CD2	TRP	A	320	32.338	18.969	18.470	1.00	28.17	C
ATOM	514	CE3	TRP	A	320	31.357	18.366	17.675	1.00	29.23	C
ATOM	515	CZ3	TRP	A	320	31.356	18.606	16.320	1.00	28.97	C
ATOM	516	CH2	TRP	A	320	32.293	19.478	15.739	1.00	28.19	C
ATOM	517	CZ2	TRP	A	320	33.260	20.086	16.492	1.00	28.61	C
ATOM	518	C	TRP	A	320	29.594	17.984	21.832	1.00	24.11	C
ATOM	519	O	TRP	A	320	28.638	18.021	21.080	1.00	23.54	O
ATOM	520	N	GLN	A	321	29.644	17.118	22.832	1.00	24.43	N
ATOM	521	CA	GLN	A	321	28.544	16.178	23.043	1.00	24.39	C
ATOM	522	CB	GLN	A	321	28.836	15.179	24.168	1.00	24.76	C
ATOM	523	CG	GLN	A	321	27.876	14.013	24.140	1.00	24.84	C
ATOM	524	CD	GLN	A	321	27.120	13.800	25.417	1.00	26.37	C
ATOM	525	OE1	GLN	A	321	27.146	14.650	26.271	1.00	29.09	O
ATOM	526	NE2	GLN	A	321	26.444	12.627	25.556	1.00	26.55	N

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ATOM	527	C	GLN	A	321	27.249	16.900	23.359	1.00	24.19	C
ATOM	528	O	GLN	A	321	26.180	16.559	22.832	1.00	24.08	O
ATOM	529	N	LEU	A	322	27.368	17.924	24.178	1.00	24.78	N
ATOM	530	CA	LEU	A	322	26.236	18.733	24.579	1.00	25.69	C
ATOM	531	CB	LEU	A	322	26.644	19.732	25.683	1.00	26.07	C
ATOM	532	CG	LEU	A	322	25.622	20.738	26.235	1.00	27.41	C
ATOM	533	CD1	LEU	A	322	24.406	20.074	26.909	1.00	29.40	C
ATOM	534	CD2	LEU	A	322	26.277	21.639	27.190	1.00	30.22	C
ATOM	535	C	LEU	A	322	25.615	19.430	23.374	1.00	26.06	C
ATOM	536	O	LEU	A	322	24.406	19.285	23.125	1.00	26.90	O
ATOM	537	N	CYS	A	323	26.420	20.140	22.587	1.00	25.58	N
ATOM	538	CA	CYS	A	323	25.893	20.774	21.384	1.00	25.11	C
ATOM	539	CB	CYS	A	323	26.996	21.554	20.686	1.00	25.72	C
ATOM	540	SG	CYS	A	323	27.607	22.944	21.675	1.00	29.20	S
ATOM	541	C	CYS	A	323	25.246	19.776	20.419	1.00	25.04	C
ATOM	542	O	CYS	A	323	24.215	20.057	19.816	1.00	23.70	O
ATOM	543	N	ALA	A	324	25.846	18.604	20.272	1.00	24.13	N
ATOM	544	CA	ALA	A	324	25.275	17.625	19.398	1.00	23.43	C
ATOM	545	CB	ALA	A	324	26.226	16.462	19.222	1.00	24.05	C
ATOM	546	C	ALA	A	324	23.913	17.141	19.912	1.00	23.43	C
ATOM	547	O	ALA	A	324	23.011	16.938	19.125	1.00	22.57	O
ATOM	548	N	ILE	A	325	23.776	16.932	21.218	1.00	23.59	N
ATOM	549	CA	ILE	A	325	22.482	16.591	21.791	1.00	24.38	C
ATOM	550	CB	ILE	A	325	22.556	16.407	23.323	1.00	24.71	C
ATOM	551	CG1	ILE	A	325	23.293	15.136	23.709	1.00	25.02	C
ATOM	552	CD1	ILE	A	325	23.649	15.149	25.190	1.00	27.28	C
ATOM	553	CG2	ILE	A	325	21.158	16.398	23.942	1.00	22.26	C
ATOM	554	C	ILE	A	325	21.479	17.705	21.501	1.00	24.86	C
ATOM	555	O	ILE	A	325	20.384	17.453	21.044	1.00	24.56	O
ATOM	556	N	LYS	A	326	21.856	18.940	21.772	1.00	25.56	N
ATOM	557	CA	LYS	A	326	20.926	20.047	21.580	1.00	26.26	C
ATOM	558	CB	LYS	A	326	21.489	21.318	22.184	1.00	26.21	C
ATOM	559	CG	LYS	A	326	21.741	21.248	23.681	1.00	29.37	C
ATOM	560	CD	LYS	A	326	20.479	20.914	24.433	1.00	33.36	C
ATOM	561	CE	LYS	A	326	20.725	20.802	25.926	1.00	36.77	C
ATOM	562	NZ	LYS	A	326	19.694	19.921	26.567	1.00	37.66	N
ATOM	563	C	LYS	A	326	20.520	20.209	20.094	1.00	26.40	C
ATOM	564	O	LYS	A	326	19.348	20.386	19.803	1.00	25.16	O
ATOM	565	N	ILE	A	327	21.480	20.110	19.175	1.00	26.86	N
ATOM	566	CA	ILE	A	327	21.208	20.174	17.740	1.00	28.16	C
ATOM	567	CB	ILE	A	327	22.511	20.235	16.930	1.00	29.15	C
ATOM	568	CG1	ILE	A	327	22.666	21.619	16.335	1.00	35.09	C
ATOM	569	CD1	ILE	A	327	23.951	21.810	15.538	1.00	39.84	C
ATOM	570	CG2	ILE	A	327	22.465	19.314	15.745	1.00	31.87	C
ATOM	571	C	ILE	A	327	20.378	19.015	17.250	1.00	27.66	C
ATOM	572	O	ILE	A	327	19.544	19.152	16.361	1.00	27.77	O
ATOM	573	N	THR	A	328	20.599	17.855	17.811	1.00	27.88	N
ATOM	574	CA	THR	A	328	19.810	16.726	17.415	1.00	28.75	C
ATOM	575	CB	THR	A	328	20.328	15.479	18.028	1.00	29.15	C
ATOM	576	OG1	THR	A	328	21.665	15.267	17.581	1.00	28.97	O
ATOM	577	CG2	THR	A	328	19.547	14.287	17.518	1.00	30.09	C
ATOM	578	C	THR	A	328	18.343	16.927	17.776	1.00	28.80	C
ATOM	579	O	THR	A	328	17.496	16.567	16.986	1.00	27.42	O
ATOM	580	N	GLU	A	329	18.051	17.530	18.928	1.00	29.14	N
ATOM	581	CA	GLU	A	329	16.658	17.852	19.278	1.00	30.60	C
ATOM	582	CB	GLU	A	329	16.546	18.559	20.643	1.00	31.73	C
ATOM	583	CG	GLU	A	329	17.198	17.863	21.820	1.00	37.45	C
ATOM	584	CD	GLU	A	329	17.178	18.684	23.122	1.00	43.70	C
ATOM	585	OE1	GLU	A	329	16.578	19.802	23.159	1.00	42.77	O
ATOM	586	OE2	GLU	A	329	17.756	18.174	24.135	1.00	49.00	O
ATOM	587	C	GLU	A	329	15.985	18.751	18.215	1.00	29.00	C
ATOM	588	O	GLU	A	329	14.864	18.502	17.776	1.00	28.96	O
ATOM	589	N	ALA	A	330	16.648	19.829	17.825	1.00	27.92	N
ATOM	590	CA	ALA	A	330	16.105	20.694	16.793	1.00	27.01	C
ATOM	591	CB	ALA	A	330	16.981	21.881	16.610	1.00	27.09	C
ATOM	592	C	ALA	A	330	15.900	19.967	15.447	1.00	27.24	C

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ATOM	593	O	ALA	A	330	14.911	20.208	14.753	1.00	27.51	O
ATOM	594	N	ILE	A	331	16.837	19.109	15.070	1.00	26.90	N
ATOM	595	CA	ILE	A	331	16.695	18.308	13.860	1.00	27.25	C
ATOM	596	CB	ILE	A	331	17.973	17.520	13.585	1.00	26.89	C
ATOM	597	CG1	ILE	A	331	19.052	18.507	13.149	1.00	27.96	C
ATOM	598	CD1	ILE	A	331	20.406	17.877	12.923	1.00	29.48	C
ATOM	599	CG2	ILE	A	331	17.766	16.414	12.484	1.00	26.39	C
ATOM	600	C	ILE	A	331	15.470	17.390	13.885	1.00	27.69	C
ATOM	601	O	ILE	A	331	14.810	17.205	12.859	1.00	27.06	O
ATOM	602	N	GLN	A	332	15.160	16.830	15.041	1.00	28.59	N
ATOM	603	CA	GLN	A	332	13.987	15.988	15.167	1.00	30.50	C
ATOM	604	CB	GLN	A	332	13.849	15.439	16.579	1.00	31.71	C
ATOM	605	CG	GLN	A	332	14.526	14.109	16.681	1.00	36.53	C
ATOM	606	CD	GLN	A	332	14.827	13.693	18.084	1.00	43.18	C
ATOM	607	OE1	GLN	A	332	14.295	14.274	19.043	1.00	46.43	O
ATOM	608	NE2	GLN	A	332	15.717	12.680	18.228	1.00	46.39	N
ATOM	609	C	GLN	A	332	12.736	16.742	14.763	1.00	30.16	C
ATOM	610	O	GLN	A	332	11.879	16.192	14.086	1.00	29.89	O
ATOM	611	N	TYR	A	333	12.666	18.012	15.142	1.00	29.91	N
ATOM	612	CA	TYR	A	333	11.548	18.863	14.773	1.00	29.79	C
ATOM	613	CB	TYR	A	333	11.552	20.152	15.632	1.00	30.02	C
ATOM	614	CG	TYR	A	333	11.052	19.929	17.038	1.00	30.98	C
ATOM	615	CD1	TYR	A	333	11.928	19.789	18.095	1.00	32.18	C
ATOM	616	CE1	TYR	A	333	11.460	19.555	19.372	1.00	34.65	C
ATOM	617	CZ	TYR	A	333	10.097	19.474	19.605	1.00	35.79	C
ATOM	618	OH	TYR	A	333	9.635	19.256	20.875	1.00	40.22	O
ATOM	619	CE2	TYR	A	333	9.207	19.621	18.590	1.00	34.47	C
ATOM	620	CD2	TYR	A	333	9.687	19.858	17.305	1.00	34.75	C
ATOM	621	C	TYR	A	333	11.543	19.187	13.272	1.00	29.21	C
ATOM	622	O	TYR	A	333	10.498	19.330	12.658	1.00	29.48	O
ATOM	623	N	VAL	A	334	12.711	19.337	12.683	1.00	28.49	N
ATOM	624	CA	VAL	A	334	12.781	19.602	11.247	1.00	28.13	C
ATOM	625	CB	VAL	A	334	14.204	20.060	10.872	1.00	28.00	C
ATOM	626	CG1	VAL	A	334	14.470	19.953	9.349	1.00	28.89	C
ATOM	627	CG2	VAL	A	334	14.441	21.427	11.401	1.00	26.70	C
ATOM	628	C	VAL	A	334	12.347	18.349	10.439	1.00	27.92	C
ATOM	629	O	VAL	A	334	11.770	18.465	9.378	1.00	26.84	O
ATOM	630	N	VAL	A	335	12.612	17.158	10.948	1.00	28.87	N
ATOM	631	CA	VAL	A	335	12.151	15.943	10.276	1.00	30.06	C
ATOM	632	CB	VAL	A	335	12.737	14.699	10.894	1.00	30.00	C
ATOM	633	CG1	VAL	A	335	12.072	13.487	10.339	1.00	32.57	C
ATOM	634	CG2	VAL	A	335	14.210	14.592	10.597	1.00	30.15	C
ATOM	635	C	VAL	A	335	10.588	15.881	10.266	1.00	30.90	C
ATOM	636	O	VAL	A	335	9.984	15.468	9.263	1.00	29.27	O
ATOM	637	N	GLU	A	336	9.953	16.356	11.344	1.00	31.20	N
ATOM	638	CA	GLU	A	336	8.489	16.425	11.393	1.00	32.50	C
ATOM	639	CB	GLU	A	336	7.961	16.735	12.812	1.00	33.25	C
ATOM	640	CG	GLU	A	336	8.283	15.671	13.862	1.00	36.91	C
ATOM	641	CD	GLU	A	336	7.627	14.299	13.616	1.00	44.18	C
ATOM	642	OE1	GLU	A	336	6.463	14.240	13.123	1.00	48.70	O
ATOM	643	OE2	GLU	A	336	8.276	13.256	13.928	1.00	47.83	O
ATOM	644	C	GLU	A	336	7.980	17.440	10.380	1.00	31.88	C
ATOM	645	O	GLU	A	336	6.994	17.194	9.697	1.00	32.26	O
ATOM	646	N	PHE	A	337	8.654	18.569	10.246	1.00	31.25	N
ATOM	647	CA	PHE	A	337	8.315	19.488	9.189	1.00	31.26	C
ATOM	648	CB	PHE	A	337	9.270	20.670	9.251	1.00	31.46	C
ATOM	649	CG	PHE	A	337	9.017	21.746	8.229	1.00	30.00	C
ATOM	650	CD1	PHE	A	337	7.842	22.467	8.237	1.00	29.18	C
ATOM	651	CE1	PHE	A	337	7.643	23.484	7.357	1.00	29.25	C
ATOM	652	CZ	PHE	A	337	8.620	23.811	6.418	1.00	30.20	C
ATOM	653	CE2	PHE	A	337	9.799	23.094	6.381	1.00	30.76	C
ATOM	654	CD2	PHE	A	337	9.988	22.059	7.287	1.00	31.21	C
ATOM	655	C	PHE	A	337	8.364	18.826	7.779	1.00	32.11	C
ATOM	656	O	PHE	A	337	7.402	18.929	7.011	1.00	31.39	O
ATOM	657	N	ALA	A	338	9.479	18.176	7.438	1.00	32.85	N
ATOM	658	CA	ALA	A	338	9.618	17.536	6.134	1.00	34.45	C

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ATOM	659	CB	ALA	A	338	10.936	16.787	6.029	1.00	34.40	C
ATOM	660	C	ALA	A	338	8.448	16.593	5.849	1.00	35.78	C
ATOM	661	O	ALA	A	338	7.848	16.667	4.806	1.00	35.41	O
ATOM	662	N	LYS	A	339	8.127	15.725	6.790	1.00	37.72	N
ATOM	663	CA	LYS	A	339	7.058	14.776	6.598	1.00	39.80	C
ATOM	664	CB	LYS	A	339	6.761	14.056	7.886	1.00	40.02	C
ATOM	665	CG	LYS	A	339	7.901	13.158	8.291	1.00	42.45	C
ATOM	666	CD	LYS	A	339	7.440	11.942	9.028	1.00	44.60	C
ATOM	667	CE	LYS	A	339	7.206	12.224	10.454	1.00	46.22	C
ATOM	668	NZ	LYS	A	339	7.415	10.966	11.174	1.00	46.80	N
ATOM	669	C	LYS	A	339	5.777	15.391	6.072	1.00	41.25	C
ATOM	670	O	LYS	A	339	5.091	14.789	5.275	1.00	41.74	O
ATOM	671	N	ARG	A	340	5.485	16.605	6.497	1.00	42.74	N
ATOM	672	CA	ARG	A	340	4.266	17.275	6.127	1.00	43.70	C
ATOM	673	CB	ARG	A	340	3.887	18.223	7.229	1.00	43.78	C
ATOM	674	CG	ARG	A	340	3.550	17.533	8.494	1.00	45.03	C
ATOM	675	CD	ARG	A	340	3.273	18.483	9.594	1.00	46.53	C
ATOM	676	NE	ARG	A	340	3.333	17.821	10.887	1.00	49.07	N
ATOM	677	CZ	ARG	A	340	2.578	18.165	11.915	1.00	51.42	C
ATOM	678	NH1	ARG	A	340	1.697	19.167	11.779	1.00	53.86	N
ATOM	679	NH2	ARG	A	340	2.691	17.510	13.063	1.00	50.56	N
ATOM	680	C	ARG	A	340	4.355	18.086	4.858	1.00	44.39	C
ATOM	681	O	ARG	A	340	3.381	18.710	4.473	1.00	44.75	O
ATOM	682	N	ILE	A	341	5.516	18.136	4.231	1.00	44.93	N
ATOM	683	CA	ILE	A	341	5.626	18.907	3.015	1.00	45.79	C
ATOM	684	CB	ILE	A	341	7.073	19.340	2.776	1.00	45.44	C
ATOM	685	CG1	ILE	A	341	7.446	20.384	3.818	1.00	45.69	C
ATOM	686	CD1	ILE	A	341	8.901	20.710	3.847	1.00	46.77	C
ATOM	687	CG2	ILE	A	341	7.240	19.881	1.357	1.00	45.67	C
ATOM	688	C	ILE	A	341	5.080	18.035	1.895	1.00	46.85	C
ATOM	689	O	ILE	A	341	5.483	16.883	1.738	1.00	46.56	O
ATOM	690	N	ASP	A	342	4.148	18.593	1.129	1.00	48.25	N
ATOM	691	CA	ASP	A	342	3.476	17.821	0.093	1.00	49.01	C
ATOM	692	CB	ASP	A	342	2.306	18.611	-0.490	1.00	50.45	C
ATOM	693	CG	ASP	A	342	1.152	18.788	0.493	1.00	53.95	C
ATOM	694	OD1	ASP	A	342	0.695	17.786	1.084	1.00	58.87	O
ATOM	695	OD2	ASP	A	342	0.636	19.914	0.713	1.00	59.55	O
ATOM	696	C	ASP	A	342	4.424	17.453	-1.031	1.00	48.01	C
ATOM	697	O	ASP	A	342	4.927	18.316	-1.747	1.00	47.92	O
ATOM	698	N	GLY	A	343	4.642	16.155	-1.185	1.00	46.69	N
ATOM	699	CA	GLY	A	343	5.544	15.642	-2.199	1.00	45.52	C
ATOM	700	C	GLY	A	343	6.710	14.888	-1.596	1.00	43.87	C
ATOM	701	O	GLY	A	343	7.268	13.970	-2.205	1.00	43.67	O
ATOM	702	N	PHE	A	344	7.045	15.232	-0.365	1.00	41.81	N
ATOM	703	CA	PHE	A	344	8.221	14.673	0.266	1.00	40.97	C
ATOM	704	CB	PHE	A	344	8.588	15.453	1.533	1.00	40.64	C
ATOM	705	CG	PHE	A	344	9.850	14.977	2.170	1.00	38.48	C
ATOM	706	CD1	PHE	A	344	11.081	15.500	1.814	1.00	36.83	C
ATOM	707	CE1	PHE	A	344	12.245	15.020	2.396	1.00	37.61	C
ATOM	708	CZ	PHE	A	344	12.190	14.000	3.311	1.00	36.20	C
ATOM	709	CE2	PHE	A	344	10.961	13.456	3.658	1.00	36.79	C
ATOM	710	CD2	PHE	A	344	9.809	13.939	3.084	1.00	36.78	C
ATOM	711	C	PHE	A	344	7.999	13.204	0.543	1.00	41.48	C
ATOM	712	O	PHE	A	344	8.864	12.366	0.254	1.00	41.42	O
ATOM	713	N	MET	A	345	6.814	12.881	1.056	1.00	42.09	N
ATOM	714	CA	MET	A	345	6.447	11.536	1.370	1.00	43.10	C
ATOM	715	CB	MET	A	345	5.247	11.496	2.326	1.00	43.84	C
ATOM	716	CG	MET	A	345	5.590	11.871	3.775	1.00	46.08	C
ATOM	717	SD	MET	A	345	7.102	11.080	4.441	1.00	50.98	S
ATOM	718	CE	MET	A	345	6.721	9.279	4.354	1.00	52.61	C
ATOM	719	C	MET	A	345	6.187	10.673	0.109	1.00	43.55	C
ATOM	720	O	MET	A	345	6.190	9.427	0.184	1.00	42.43	O
ATOM	721	N	GLU	A	346	5.974	11.311	-1.040	1.00	44.36	N
ATOM	722	CA	GLU	A	346	5.839	10.568	-2.291	1.00	45.64	C
ATOM	723	CB	GLU	A	346	5.107	11.384	-3.339	1.00	46.00	C
ATOM	724	CG	GLU	A	346	3.616	11.455	-3.132	1.00	49.03	C

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ATOM	725	CD	GLU	A	346	2.989	12.662	-3.821	1.00	54.25	C
ATOM	726	OE1	GLU	A	346	3.726	13.555	-4.328	1.00	56.30	O
ATOM	727	OE2	GLU	A	346	1.740	12.718	-3.852	1.00	58.05	O
ATOM	728	C	GLU	A	346	7.182	10.143	-2.901	1.00	45.79	C
ATOM	729	O	GLU	A	346	7.209	9.327	-3.826	1.00	46.33	O
ATOM	730	N	LEU	A	347	8.288	10.691	-2.411	1.00	45.30	N
ATOM	731	CA	LEU	A	347	9.593	10.361	-2.983	1.00	44.95	C
ATOM	732	CB	LEU	A	347	10.618	11.445	-2.650	1.00	44.65	C
ATOM	733	CG	LEU	A	347	10.252	12.868	-3.077	1.00	44.22	C
ATOM	734	CD1	LEU	A	347	11.065	13.905	-2.341	1.00	43.57	C
ATOM	735	CD2	LEU	A	347	10.447	13.049	-4.576	1.00	44.47	C
ATOM	736	C	LEU	A	347	10.086	9.010	-2.469	1.00	44.60	C
ATOM	737	O	LEU	A	347	9.634	8.530	-1.426	1.00	43.99	O
ATOM	738	N	CYS	A	348	11.007	8.392	-3.205	1.00	44.39	N
ATOM	739	CA	CYS	A	348	11.599	7.132	-2.754	1.00	44.78	C
ATOM	740	CB	CYS	A	348	12.511	6.526	-3.835	1.00	44.94	C
ATOM	741	SG	CYS	A	348	13.860	7.612	-4.385	1.00	48.13	S
ATOM	742	C	CYS	A	348	12.388	7.401	-1.474	1.00	43.97	C
ATOM	743	O	CYS	A	348	12.982	8.475	-1.326	1.00	42.90	O
ATOM	744	N	GLN	A	349	12.401	6.427	-0.567	1.00	43.70	N
ATOM	745	CA	GLN	A	349	13.096	6.569	0.708	1.00	44.41	C
ATOM	746	CB	GLN	A	349	13.178	5.250	1.487	1.00	45.15	C
ATOM	747	CG	GLN	A	349	13.587	5.479	2.949	1.00	47.77	C
ATOM	748	CD	GLN	A	349	13.747	4.207	3.723	1.00	51.04	C
ATOM	749	OE1	GLN	A	349	13.880	3.124	3.139	1.00	53.73	O
ATOM	750	NE2	GLN	A	349	13.761	4.325	5.040	1.00	53.95	N
ATOM	751	C	GLN	A	349	14.499	7.124	0.495	1.00	43.84	C
ATOM	752	O	GLN	A	349	15.017	7.862	1.324	1.00	43.52	O
ATOM	753	N	ASN	A	350	15.106	6.753	-0.623	1.00	43.26	N
ATOM	754	CA	ASN	A	350	16.451	7.175	-0.929	1.00	43.16	C
ATOM	755	CB	ASN	A	350	16.936	6.460	-2.175	1.00	43.98	C
ATOM	756	CG	ASN	A	350	16.970	4.940	-1.994	1.00	48.26	C
ATOM	757	OD1	ASN	A	350	18.058	4.340	-1.904	1.00	52.77	O
ATOM	758	ND2	ASN	A	350	15.773	4.305	-1.934	1.00	51.57	N
ATOM	759	C	ASN	A	350	16.563	8.686	-1.116	1.00	40.98	C
ATOM	760	O	ASN	A	350	17.499	9.296	-0.637	1.00	40.25	O
ATOM	761	N	ASP	A	351	15.638	9.266	-1.860	1.00	39.10	N
ATOM	762	CA	ASP	A	351	15.643	10.696	-2.065	1.00	38.32	C
ATOM	763	CB	ASP	A	351	14.794	11.100	-3.253	1.00	38.60	C
ATOM	764	CG	ASP	A	351	15.504	10.847	-4.590	1.00	41.32	C
ATOM	765	OD1	ASP	A	351	16.656	10.309	-4.587	1.00	42.06	O
ATOM	766	OD2	ASP	A	351	14.977	11.143	-5.686	1.00	42.98	O
ATOM	767	C	ASP	A	351	15.194	11.404	-0.783	1.00	36.92	C
ATOM	768	O	ASP	A	351	15.721	12.435	-0.464	1.00	35.52	O
ATOM	769	N	GLN	A	352	14.279	10.813	-0.023	1.00	35.97	N
ATOM	770	CA	GLN	A	352	13.905	11.377	1.265	1.00	35.61	C
ATOM	771	CB	GLN	A	352	12.875	10.478	1.950	1.00	35.48	C
ATOM	772	CG	GLN	A	352	11.497	10.599	1.322	1.00	37.95	C
ATOM	773	CD	GLN	A	352	10.561	9.498	1.737	1.00	40.62	C
ATOM	774	OE1	GLN	A	352	10.668	8.974	2.839	1.00	40.95	O
ATOM	775	NE2	GLN	A	352	9.649	9.123	0.848	1.00	44.80	N
ATOM	776	C	GLN	A	352	15.154	11.554	2.137	1.00	34.57	C
ATOM	777	O	GLN	A	352	15.388	12.611	2.720	1.00	32.40	O
ATOM	778	N	ILE	A	353	15.970	10.508	2.184	1.00	33.88	N
ATOM	779	CA	ILE	A	353	17.178	10.487	3.002	1.00	34.01	C
ATOM	780	CB	ILE	A	353	17.772	9.049	2.998	1.00	33.98	C
ATOM	781	CG1	ILE	A	353	16.805	8.112	3.715	1.00	36.61	C
ATOM	782	CD1	ILE	A	353	17.075	6.631	3.477	1.00	38.26	C
ATOM	783	CG2	ILE	A	353	19.101	9.002	3.715	1.00	34.10	C
ATOM	784	C	ILE	A	353	18.225	11.498	2.548	1.00	32.99	C
ATOM	785	O	ILE	A	353	18.821	12.187	3.364	1.00	32.18	O
ATOM	786	N	VAL	A	354	18.466	11.563	1.246	1.00	31.86	N
ATOM	787	CA	VAL	A	354	19.433	12.515	0.698	1.00	31.38	C
ATOM	788	CB	VAL	A	354	19.569	12.320	-0.821	1.00	31.50	C
ATOM	789	CG1	VAL	A	354	20.148	13.516	-1.458	1.00	31.80	C
ATOM	790	CG2	VAL	A	354	20.388	11.039	-1.149	1.00	32.45	C

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ATOM	791	C	VAL	A	354	19.066	13.988	0.998	1.00	29.81	C
ATOM	792	O	VAL	A	354	19.939	14.794	1.317	1.00	29.46	O
ATOM	793	N	LEU	A	355	17.780	14.316	0.901	1.00	28.52	N
ATOM	794	CA	LEU	A	355	17.317	15.673	1.175	1.00	27.57	C
ATOM	795	CB	LEU	A	355	15.867	15.859	0.755	1.00	27.23	C
ATOM	796	CG	LEU	A	355	15.593	15.830	-0.741	1.00	27.16	C
ATOM	797	CD1	LEU	A	355	14.104	15.935	-0.931	1.00	28.72	C
ATOM	798	CD2	LEU	A	355	16.337	16.878	-1.514	1.00	26.89	C
ATOM	799	C	LEU	A	355	17.435	16.028	2.642	1.00	26.38	C
ATOM	800	O	LEU	A	355	17.724	17.171	2.969	1.00	24.91	O
ATOM	801	N	LEU	A	356	17.184	15.067	3.522	1.00	26.87	N
ATOM	802	CA	LEU	A	356	17.330	15.291	4.962	1.00	28.02	C
ATOM	803	CB	LEU	A	356	16.567	14.232	5.788	1.00	28.75	C
ATOM	804	CG	LEU	A	356	15.046	14.442	5.700	1.00	31.27	C
ATOM	805	CD1	LEU	A	356	14.317	13.319	6.329	1.00	33.71	C
ATOM	806	CD2	LEU	A	356	14.608	15.740	6.323	1.00	31.98	C
ATOM	807	C	LEU	A	356	18.785	15.340	5.404	1.00	27.73	C
ATOM	808	O	LEU	A	356	19.138	16.160	6.234	1.00	27.81	O
ATOM	809	N	LYS	A	357	19.631	14.463	4.891	1.00	28.00	N
ATOM	810	CA	LYS	A	357	21.038	14.523	5.263	1.00	29.47	C
ATOM	811	CB	LYS	A	357	21.875	13.426	4.613	1.00	29.39	C
ATOM	812	CG	LYS	A	357	21.562	12.033	5.037	1.00	33.92	C
ATOM	813	CD	LYS	A	357	22.586	11.034	4.457	1.00	37.74	C
ATOM	814	CE	LYS	A	357	22.683	9.804	5.331	1.00	41.03	C
ATOM	815	NZ	LYS	A	357	23.255	8.598	4.607	1.00	43.01	N
ATOM	816	C	LYS	A	357	21.600	15.853	4.830	1.00	29.89	C
ATOM	817	O	LYS	A	357	22.382	16.444	5.542	1.00	30.98	O
ATOM	818	N	ALA	A	358	21.207	16.338	3.657	1.00	30.12	N
ATOM	819	CA	ALA	A	358	21.750	17.612	3.181	1.00	30.98	C
ATOM	820	CB	ALA	A	358	21.753	17.654	1.658	1.00	31.73	C
ATOM	821	C	ALA	A	358	21.056	18.857	3.702	1.00	30.81	C
ATOM	822	O	ALA	A	358	21.686	19.893	3.875	1.00	33.30	O
ATOM	823	N	GLY	A	359	19.765	18.777	3.940	1.00	29.32	N
ATOM	824	CA	GLY	A	359	19.040	19.938	4.331	1.00	28.50	C
ATOM	825	C	GLY	A	359	18.606	20.119	5.764	1.00	27.82	C
ATOM	826	O	GLY	A	359	18.236	21.223	6.110	1.00	27.60	O
ATOM	827	N	SER	A	360	18.630	19.089	6.591	1.00	26.28	N
ATOM	828	CA	SER	A	360	18.064	19.239	7.905	1.00	26.79	C
ATOM	829	CB	SER	A	360	17.984	17.889	8.631	1.00	27.01	C
ATOM	830	OG	SER	A	360	19.287	17.372	8.858	1.00	30.95	O
ATOM	831	C	SER	A	360	18.786	20.315	8.699	1.00	26.61	C
ATOM	832	O	SER	A	360	18.139	21.164	9.310	1.00	26.71	O
ATOM	833	N	LEU	A	361	20.116	20.345	8.635	1.00	26.46	N
ATOM	834	CA	LEU	A	361	20.887	21.373	9.338	1.00	26.75	C
ATOM	835	CB	LEU	A	361	22.380	21.042	9.306	1.00	26.79	C
ATOM	836	CG	LEU	A	361	23.250	21.762	10.334	1.00	28.75	C
ATOM	837	CD1	LEU	A	361	22.803	21.528	11.780	1.00	28.83	C
ATOM	838	CD2	LEU	A	361	24.747	21.342	10.154	1.00	30.56	C
ATOM	839	C	LEU	A	361	20.660	22.765	8.782	1.00	26.67	C
ATOM	840	O	LEU	A	361	20.593	23.740	9.545	1.00	26.63	O
ATOM	841	N	GLU	A	362	20.550	22.885	7.468	1.00	25.93	N
ATOM	842	CA	GLU	A	362	20.258	24.192	6.875	1.00	26.57	C
ATOM	843	CB	GLU	A	362	20.158	24.122	5.357	1.00	26.98	C
ATOM	844	CG	GLU	A	362	21.329	23.433	4.674	1.00	31.21	C
ATOM	845	CD	GLU	A	362	21.206	23.396	3.149	1.00	37.21	C
ATOM	846	OE1	GLU	A	362	22.086	22.796	2.478	1.00	41.59	O
ATOM	847	OE2	GLU	A	362	20.212	23.932	2.619	1.00	43.73	O
ATOM	848	C	GLU	A	362	18.931	24.726	7.430	1.00	25.89	C
ATOM	849	O	GLU	A	362	18.823	25.921	7.697	1.00	24.74	O
ATOM	850	N	VAL	A	363	17.920	23.868	7.592	1.00	25.19	N
ATOM	851	CA	VAL	A	363	16.647	24.362	8.112	1.00	26.09	C
ATOM	852	CB	VAL	A	363	15.494	23.356	7.990	1.00	25.99	C
ATOM	853	CG1	VAL	A	363	14.256	23.894	8.658	1.00	27.49	C
ATOM	854	CG2	VAL	A	363	15.182	23.075	6.538	1.00	27.46	C
ATOM	855	C	VAL	A	363	16.815	24.781	9.574	1.00	25.70	C
ATOM	856	O	VAL	A	363	16.210	25.732	10.020	1.00	25.15	O

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ATOM	857	N	VAL	A	364	17.682	24.091	10.308	1.00	26.29	N
ATOM	858	CA	VAL	A	364	17.942	24.451	11.690	1.00	25.82	C
ATOM	859	CB	VAL	A	364	18.867	23.435	12.363	1.00	26.43	C
ATOM	860	CG1	VAL	A	364	19.315	23.910	13.716	1.00	25.43	C
ATOM	861	CG2	VAL	A	364	18.171	22.105	12.538	1.00	27.04	C
ATOM	862	C	VAL	A	364	18.528	25.865	11.747	1.00	26.05	O
ATOM	863	O	VAL	A	364	18.110	26.692	12.570	1.00	25.23	N
ATOM	864	N	PHE	A	365	19.491	26.162	10.877	1.00	25.43	C
ATOM	865	CA	PHE	A	365	20.098	27.491	10.897	1.00	25.79	C
ATOM	866	CB	PHE	A	365	21.372	27.506	10.102	1.00	26.05	C
ATOM	867	CG	PHE	A	365	22.482	26.755	10.743	1.00	26.79	C
ATOM	868	CD1	PHE	A	365	22.830	26.990	12.046	1.00	28.32	C
ATOM	869	CE1	PHE	A	365	23.869	26.329	12.628	1.00	29.90	C
ATOM	870	CZ	PHE	A	365	24.601	25.430	11.894	1.00	31.06	C
ATOM	871	CE2	PHE	A	365	24.290	25.215	10.614	1.00	30.47	C
ATOM	872	CD2	PHE	A	365	23.226	25.886	10.024	1.00	29.26	C
ATOM	873	C	PHE	A	365	19.157	28.591	10.418	1.00	26.05	O
ATOM	874	O	PHE	A	365	19.265	29.745	10.846	1.00	26.08	N
ATOM	875	N	ILE	A	366	18.213	28.242	9.554	1.00	26.60	C
ATOM	876	CA	ILE	A	366	17.183	29.194	9.178	1.00	27.03	C
ATOM	877	CB	ILE	A	366	16.365	28.719	7.970	1.00	27.55	C
ATOM	878	CG1	ILE	A	366	17.273	28.657	6.731	1.00	27.31	C
ATOM	879	CD1	ILE	A	366	16.641	28.018	5.520	1.00	26.80	C
ATOM	880	CG2	ILE	A	366	15.179	29.670	7.720	1.00	27.78	C
ATOM	881	C	ILE	A	366	16.325	29.422	10.404	1.00	26.64	O
ATOM	882	O	ILE	A	366	16.186	30.523	10.833	1.00	27.09	N
ATOM	883	N	ARG	A	367	15.792	28.375	11.009	1.00	27.45	C
ATOM	884	CA	ARG	A	367	14.990	28.542	12.229	1.00	27.84	C
ATOM	885	CB	ARG	A	367	14.500	27.204	12.733	1.00	27.21	C
ATOM	886	CG	ARG	A	367	13.501	26.572	11.840	1.00	27.21	C
ATOM	887	CD	ARG	A	367	12.989	25.262	12.377	1.00	26.26	C
ATOM	888	NE	ARG	A	367	11.797	24.825	11.687	1.00	27.92	N
ATOM	889	CZ	ARG	A	367	11.017	23.827	12.095	1.00	30.29	C
ATOM	890	NH1	ARG	A	367	11.308	23.140	13.190	1.00	30.75	N
ATOM	891	NH2	ARG	A	367	9.933	23.529	11.412	1.00	31.09	N
ATOM	892	C	ARG	A	367	15.723	29.268	13.367	1.00	28.32	C
ATOM	893	O	ARG	A	367	15.104	29.904	14.228	1.00	28.51	O
ATOM	894	N	MET	A	368	17.038	29.172	13.374	1.00	29.28	N
ATOM	895	CA	MET	A	368	17.832	29.887	14.359	1.00	30.61	C
ATOM	896	CB	MET	A	368	19.311	29.754	14.039	1.00	30.32	C
ATOM	897	CG	MET	A	368	20.188	30.279	15.100	1.00	30.51	C
ATOM	898	SD	MET	A	368	21.905	29.966	14.792	1.00	31.75	S
ATOM	899	CE	MET	A	368	22.107	30.986	13.388	1.00	33.23	C
ATOM	900	C	MET	A	368	17.484	31.372	14.427	1.00	31.27	C
ATOM	901	O	MET	A	368	17.590	31.982	15.481	1.00	31.35	O
ATOM	902	N	CYS	A	369	17.074	31.963	13.328	1.00	32.36	N
ATOM	903	CA	CYS	A	369	16.775	33.385	13.375	1.00	34.85	C
ATOM	904	CB	CYS	A	369	16.614	34.005	11.987	1.00	35.08	C
ATOM	905	SG	CYS	A	369	15.048	33.719	11.195	1.00	41.49	S
ATOM	906	C	CYS	A	369	15.601	33.738	14.286	1.00	34.66	C
ATOM	907	O	CYS	A	369	15.556	34.844	14.785	1.00	36.34	O
ATOM	908	N	ARG	A	370	14.705	32.794	14.569	1.00	33.99	N
ATOM	909	CA	ARG	A	370	13.589	33.045	15.460	1.00	32.77	C
ATOM	910	CB	ARG	A	370	12.559	31.933	15.319	1.00	32.42	C
ATOM	911	CG	ARG	A	370	12.173	31.608	13.890	1.00	32.81	C
ATOM	912	CD	ARG	A	370	11.507	30.270	13.790	1.00	33.89	C
ATOM	913	NE	ARG	A	370	10.153	30.290	14.304	1.00	32.17	N
ATOM	914	CZ	ARG	A	370	9.752	29.738	15.412	1.00	32.53	C
ATOM	915	NH1	ARG	A	370	10.598	29.098	16.193	1.00	35.61	N
ATOM	916	NH2	ARG	A	370	8.472	29.815	15.748	1.00	33.49	N
ATOM	917	C	ARG	A	370	14.051	33.036	16.912	1.00	32.83	O
ATOM	918	O	ARG	A	370	13.322	33.465	17.817	1.00	32.92	C
ATOM	919	N	ALA	A	371	15.241	32.488	17.131	1.00	31.07	N
ATOM	920	CA	ALA	A	371	15.757	32.294	18.455	1.00	29.60	C
ATOM	921	CB	ALA	A	371	15.928	30.792	18.720	1.00	29.76	C
ATOM	922	C	ALA	A	371	17.077	33.001	18.554	1.00	28.59	C

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ATOM	923	O	ALA	A	371	17.964	32.561	19.226	1.00	27.57	O
ATOM	924	N	PHE	A	372	17.198	34.127	17.888	1.00	28.91	N
ATOM	925	CA	PHE	A	372	18.452	34.836	17.848	1.00	28.90	C
ATOM	926	CB	PHE	A	372	19.079	34.660	16.480	1.00	28.04	C
ATOM	927	CG	PHE	A	372	20.485	35.112	16.406	1.00	27.18	C
ATOM	928	CD1	PHE	A	372	21.515	34.231	16.614	1.00	28.47	C
ATOM	929	CE1	PHE	A	372	22.829	34.661	16.546	1.00	30.76	C
ATOM	930	CZ	PHE	A	372	23.107	36.004	16.312	1.00	28.92	C
ATOM	931	CE2	PHE	A	372	22.085	36.873	16.119	1.00	28.65	C
ATOM	932	CD2	PHE	A	372	20.781	36.429	16.158	1.00	27.09	C
ATOM	933	C	PHE	A	372	18.202	36.304	18.127	1.00	30.17	C
ATOM	934	O	PHE	A	372	17.312	36.889	17.543	1.00	30.94	O
ATOM	935	N	ASP	A	373	19.005	36.885	19.000	1.00	31.57	N
ATOM	936	CA	ASP	A	373	18.910	38.293	19.376	1.00	33.31	C
ATOM	937	CB	ASP	A	373	19.058	38.438	20.900	1.00	33.82	C
ATOM	938	CG	ASP	A	373	18.989	39.902	21.381	1.00	36.02	C
ATOM	939	OD1	ASP	A	373	18.985	40.818	20.530	1.00	41.04	O
ATOM	940	OD2	ASP	A	373	18.972	40.227	22.591	1.00	36.84	O
ATOM	941	C	ASP	A	373	20.020	39.049	18.649	1.00	34.95	C
ATOM	942	O	ASP	A	373	21.198	39.063	19.064	1.00	34.64	O
ATOM	943	N	SER	A	374	19.636	39.678	17.553	1.00	36.75	N
ATOM	944	CA	SER	A	374	20.585	40.409	16.717	1.00	39.28	C
ATOM	945	CB	SER	A	374	19.866	40.916	15.474	1.00	39.26	C
ATOM	946	OG	SER	A	374	20.836	41.201	14.487	1.00	43.88	O
ATOM	947	C	SER	A	374	21.325	41.581	17.378	1.00	39.94	C
ATOM	948	O	SER	A	374	22.515	41.766	17.173	1.00	40.56	O
ATOM	949	N	GLN	A	375	20.626	42.366	18.186	1.00	41.01	N
ATOM	950	CA	GLN	A	375	21.239	43.516	18.810	1.00	41.65	C
ATOM	951	CB	GLN	A	375	20.197	44.362	19.565	1.00	42.91	C
ATOM	952	CG	GLN	A	375	18.913	44.675	18.767	1.00	47.27	C
ATOM	953	CD	GLN	A	375	18.116	45.864	19.353	1.00	53.49	C
ATOM	954	OE1	GLN	A	375	18.626	46.997	19.399	1.00	57.17	O
ATOM	955	NE2	GLN	A	375	16.877	45.608	19.788	1.00	54.72	N
ATOM	956	C	GLN	A	375	22.344	43.098	19.762	1.00	40.86	C
ATOM	957	O	GLN	A	375	23.365	43.773	19.858	1.00	41.50	O
ATOM	958	N	ASN	A	376	22.155	41.987	20.463	1.00	39.20	N
ATOM	959	CA	ASN	A	376	23.137	41.552	21.441	1.00	38.16	C
ATOM	960	CB	ASN	A	376	22.438	41.264	22.766	1.00	38.40	C
ATOM	961	CG	ASN	A	376	21.791	42.527	23.387	1.00	40.33	C
ATOM	962	OD1	ASN	A	376	22.488	43.368	23.935	1.00	41.58	O
ATOM	963	ND2	ASN	A	376	20.452	42.644	23.301	1.00	40.49	N
ATOM	964	C	ASN	A	376	24.019	40.360	21.002	1.00	36.51	C
ATOM	965	O	ASN	A	376	24.852	39.906	21.769	1.00	37.34	O
ATOM	966	N	ASN	A	377	23.840	39.859	19.789	1.00	33.92	N
ATOM	967	CA	ASN	A	377	24.632	38.727	19.284	1.00	32.39	C
ATOM	968	CB	ASN	A	377	26.094	39.138	19.079	1.00	31.52	C
ATOM	969	CG	ASN	A	377	26.772	38.334	17.993	1.00	31.73	C
ATOM	970	OD1	ASN	A	377	26.142	37.995	16.998	1.00	33.03	O
ATOM	971	ND2	ASN	A	377	28.050	38.007	18.176	1.00	27.90	N
ATOM	972	C	ASN	A	377	24.550	37.477	20.194	1.00	31.00	C
ATOM	973	O	ASN	A	377	25.560	37.005	20.708	1.00	31.17	O
ATOM	974	N	THR	A	378	23.336	36.976	20.410	1.00	29.28	N
ATOM	975	CA	THR	A	378	23.110	35.831	21.282	1.00	28.19	C
ATOM	976	CB	THR	A	378	22.643	36.241	22.727	1.00	29.06	C
ATOM	977	OG1	THR	A	378	21.395	36.949	22.674	1.00	27.46	O
ATOM	978	CG2	THR	A	378	23.663	37.127	23.462	1.00	28.26	C
ATOM	979	C	THR	A	378	22.070	34.895	20.708	1.00	26.71	C
ATOM	980	O	THR	A	378	21.139	35.318	20.011	1.00	26.15	O
ATOM	981	N	VAL	A	379	22.231	33.615	21.032	1.00	26.22	N
ATOM	982	CA	VAL	A	379	21.361	32.557	20.517	1.00	24.86	C
ATOM	983	CB	VAL	A	379	22.149	31.671	19.525	1.00	24.33	C
ATOM	984	CG1	VAL	A	379	23.217	30.881	20.210	1.00	24.14	C
ATOM	985	CG2	VAL	A	379	21.210	30.747	18.777	1.00	24.47	C
ATOM	986	C	VAL	A	379	20.815	31.711	21.637	1.00	24.23	C
ATOM	987	O	VAL	A	379	21.507	31.421	22.559	1.00	24.32	O
ATOM	988	N	TYR	A	380	19.569	31.283	21.519	1.00	24.94	N



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ATOM	989	CA	TYR	A	380	18.905	30.450	22.506	1.00	25.03	C
ATOM	990	CB	TYR	A	380	17.410	30.313	22.141	1.00	24.86	C
ATOM	991	CG	TYR	A	380	16.514	29.758	23.215	1.00	27.20	C
ATOM	992	CD1	TYR	A	380	16.614	30.197	24.535	1.00	32.61	C
ATOM	993	CE1	TYR	A	380	15.799	29.705	25.521	1.00	32.61	C
ATOM	994	CZ	TYR	A	380	14.852	28.746	25.210	1.00	35.82	C
ATOM	995	OH	TYR	A	380	14.038	28.236	26.193	1.00	38.69	O
ATOM	996	CE2	TYR	A	380	14.742	28.277	23.938	1.00	34.16	C
ATOM	997	CD2	TYR	A	380	15.589	28.791	22.939	1.00	32.66	C
ATOM	998	C	TYR	A	380	19.589	29.086	22.523	1.00	25.13	C
ATOM	999	O	TYR	A	380	19.647	28.416	21.514	1.00	25.44	O
ATOM	1000	N	PHE	A	381	20.127	28.698	23.675	1.00	25.96	N
ATOM	1001	CA	PHE	A	381	20.902	27.470	23.824	1.00	25.59	C
ATOM	1002	CB	PHE	A	381	22.328	27.773	23.471	1.00	25.60	C
ATOM	1003	CG	PHE	A	381	23.263	26.709	23.828	1.00	25.28	C
ATOM	1004	CD1	PHE	A	381	23.306	25.561	23.106	1.00	26.68	C
ATOM	1005	CE1	PHE	A	381	24.190	24.559	23.454	1.00	29.89	C
ATOM	1006	CZ	PHE	A	381	25.049	24.733	24.537	1.00	28.60	C
ATOM	1007	CE2	PHE	A	381	25.007	25.865	25.234	1.00	28.13	C
ATOM	1008	CD2	PHE	A	381	24.107	26.851	24.895	1.00	27.85	C
ATOM	1009	C	PHE	A	381	20.879	26.914	25.251	1.00	26.62	C
ATOM	1010	O	PHE	A	381	21.215	27.604	26.209	1.00	26.25	O
ATOM	1011	N	ASP	A	382	20.481	25.664	25.416	1.00	27.37	N
ATOM	1012	CA	ASP	A	382	20.441	25.075	26.766	1.00	28.62	C
ATOM	1013	CB	ASP	A	382	21.885	24.760	27.242	1.00	28.80	C
ATOM	1014	CG	ASP	A	382	21.936	23.653	28.283	1.00	31.74	C
ATOM	1015	OD1	ASP	A	382	20.973	22.859	28.374	1.00	34.71	O
ATOM	1016	OD2	ASP	A	382	22.911	23.477	29.045	1.00	34.98	O
ATOM	1017	C	ASP	A	382	19.705	25.888	27.853	1.00	28.15	C
ATOM	1018	O	ASP	A	382	20.150	25.923	28.997	1.00	29.36	O
ATOM	1019	N	GLY	A	383	18.564	26.485	27.514	1.00	28.44	N
ATOM	1020	CA	GLY	A	383	17.770	27.238	28.488	1.00	28.32	C
ATOM	1021	C	GLY	A	383	17.958	28.758	28.594	1.00	27.86	C
ATOM	1022	O	GLY	A	383	17.144	29.476	29.196	1.00	29.11	O
ATOM	1023	N	LYS	A	384	19.032	29.289	28.033	1.00	26.62	N
ATOM	1024	CA	LYS	A	384	19.241	30.731	28.108	1.00	26.42	C
ATOM	1025	CB	LYS	A	384	20.185	31.068	29.267	1.00	26.08	C
ATOM	1026	CG	LYS	A	384	19.627	30.747	30.653	1.00	28.51	C
ATOM	1027	CD	LYS	A	384	20.486	31.424	31.751	1.00	29.39	C
ATOM	1028	CE	LYS	A	384	20.028	31.086	33.196	1.00	30.70	C
ATOM	1029	NZ	LYS	A	384	20.910	31.746	34.288	1.00	29.22	N
ATOM	1030	C	LYS	A	384	19.797	31.259	26.791	1.00	25.94	C
ATOM	1031	O	LYS	A	384	20.097	30.466	25.900	1.00	26.76	O
ATOM	1032	N	TYR	A	385	19.974	32.578	26.672	1.00	24.63	N
ATOM	1033	CA	TYR	A	385	20.572	33.145	25.466	1.00	24.57	C
ATOM	1034	CB	TYR	A	385	19.948	34.488	25.115	1.00	24.03	C
ATOM	1035	CG	TYR	A	385	18.685	34.353	24.311	1.00	24.39	C
ATOM	1036	CD1	TYR	A	385	17.468	34.095	24.917	1.00	26.02	C
ATOM	1037	CE1	TYR	A	385	16.320	34.000	24.163	1.00	26.31	C
ATOM	1038	CZ	TYR	A	385	16.411	34.121	22.799	1.00	28.74	C
ATOM	1039	OH	TYR	A	385	15.321	33.976	21.988	1.00	27.24	O
ATOM	1040	CE2	TYR	A	385	17.628	34.353	22.195	1.00	26.89	C
ATOM	1041	CD2	TYR	A	385	18.723	34.458	22.944	1.00	24.65	C
ATOM	1042	C	TYR	A	385	22.101	33.213	25.671	1.00	24.69	C
ATOM	1043	O	TYR	A	385	22.590	33.626	26.720	1.00	25.62	O
ATOM	1044	N	ALA	A	386	22.825	32.741	24.671	1.00	24.40	N
ATOM	1045	CA	ALA	A	386	24.254	32.515	24.738	1.00	24.38	C
ATOM	1046	CB	ALA	A	386	24.514	31.107	24.385	1.00	23.79	C
ATOM	1047	C	ALA	A	386	25.008	33.368	23.745	1.00	25.29	C
ATOM	1048	O	ALA	A	386	24.623	33.438	22.579	1.00	26.61	O
ATOM	1049	N	SER	A	387	26.085	33.976	24.209	1.00	25.98	N
ATOM	1050	CA	SER	A	387	27.031	34.711	23.369	1.00	26.98	C
ATOM	1051	CB	SER	A	387	27.840	35.628	24.236	1.00	26.78	C
ATOM	1052	OG	SER	A	387	28.416	34.847	25.267	1.00	30.72	O
ATOM	1053	C	SER	A	387	27.985	33.696	22.787	1.00	27.67	C
ATOM	1054	O	SER	A	387	27.984	32.548	23.233	1.00	26.96	O

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ATOM	1055	N	PRO	A	388	28.776	34.084	21.785	1.00	28.55	N
ATOM	1056	CA	PRO	A	388	29.788	33.193	21.216	1.00	29.40	C
ATOM	1057	CB	PRO	A	388	30.510	34.088	20.180	1.00	29.67	C
ATOM	1058	CG	PRO	A	388	29.538	35.118	19.839	1.00	29.41	C
ATOM	1059	CD	PRO	A	388	28.781	35.393	21.107	1.00	29.03	C
ATOM	1060	C	PRO	A	388	30.775	32.659	22.250	1.00	30.29	C
ATOM	1061	O	PRO	A	388	31.346	31.581	22.052	1.00	30.55	O
ATOM	1062	N	ASP	A	389	30.972	33.389	23.338	1.00	31.61	N
ATOM	1063	CA	ASP	A	389	31.864	32.951	24.406	1.00	32.74	C
ATOM	1064	CB	ASP	A	389	31.882	33.986	25.510	1.00	34.07	C
ATOM	1065	CG	ASP	A	389	32.640	35.207	25.127	1.00	39.93	C
ATOM	1066	OD1	ASP	A	389	33.325	35.175	24.070	1.00	47.04	O
ATOM	1067	OD2	ASP	A	389	32.601	36.259	25.813	1.00	46.60	O
ATOM	1068	C	ASP	A	389	31.484	31.614	25.044	1.00	31.53	C
ATOM	1069	O	ASP	A	389	32.359	30.893	25.528	1.00	31.63	O
ATOM	1070	N	VAL	A	390	30.189	31.317	25.069	1.00	29.87	N
ATOM	1071	CA	VAL	A	390	29.667	30.079	25.616	1.00	29.20	C
ATOM	1072	CB	VAL	A	390	28.119	30.083	25.572	1.00	29.33	C
ATOM	1073	CG1	VAL	A	390	27.579	28.705	25.643	1.00	29.50	C
ATOM	1074	CG2	VAL	A	390	27.582	30.907	26.704	1.00	29.08	C
ATOM	1075	C	VAL	A	390	30.183	28.865	24.870	1.00	28.35	C
ATOM	1076	O	VAL	A	390	30.307	27.811	25.440	1.00	28.58	O
ATOM	1077	N	PHE	A	391	30.551	29.038	23.610	1.00	28.30	N
ATOM	1078	CA	PHE	A	391	31.038	27.943	22.785	1.00	27.98	C
ATOM	1079	CB	PHE	A	391	30.365	28.034	21.431	1.00	27.73	C
ATOM	1080	CG	PHE	A	391	28.882	28.039	21.514	1.00	26.60	C
ATOM	1081	CD1	PHE	A	391	28.180	29.233	21.549	1.00	25.13	C
ATOM	1082	CE1	PHE	A	391	26.814	29.228	21.640	1.00	24.90	C
ATOM	1083	CZ	PHE	A	391	26.129	28.025	21.674	1.00	24.94	C
ATOM	1084	CE2	PHE	A	391	26.812	26.837	21.650	1.00	24.26	C
ATOM	1085	CD2	PHE	A	391	28.180	26.840	21.574	1.00	25.61	C
ATOM	1086	C	PHE	A	391	32.566	27.838	22.571	1.00	28.31	C
ATOM	1087	O	PHE	A	391	33.018	27.054	21.729	1.00	27.05	O
ATOM	1088	N	LYS	A	392	33.328	28.579	23.356	1.00	29.26	N
ATOM	1089	CA	LYS	A	392	34.795	28.578	23.281	1.00	31.34	C
ATOM	1090	CB	LYS	A	392	35.366	29.495	24.377	1.00	32.61	C
ATOM	1091	CG	LYS	A	392	36.861	29.771	24.281	1.00	35.79	C
ATOM	1092	CD	LYS	A	392	37.301	30.620	25.474	1.00	39.49	C
ATOM	1093	CE	LYS	A	392	38.826	30.579	25.699	1.00	41.94	C
ATOM	1094	NZ	LYS	A	392	39.185	31.071	27.075	1.00	42.28	N
ATOM	1095	C	LYS	A	392	35.456	27.202	23.366	1.00	31.54	C
ATOM	1096	O	LYS	A	392	36.322	26.898	22.567	1.00	31.50	O
ATOM	1097	N	SER	A	393	35.008	26.343	24.288	1.00	32.67	N
ATOM	1098	CA	SER	A	393	35.571	25.003	24.431	1.00	32.44	C
ATOM	1099	CB	SER	A	393	34.989	24.270	25.624	1.00	32.78	C
ATOM	1100	OG	SER	A	393	35.056	25.069	26.784	1.00	35.03	O
ATOM	1101	C	SER	A	393	35.400	24.110	23.240	1.00	32.29	C
ATOM	1102	O	SER	A	393	36.048	23.062	23.169	1.00	32.31	O
ATOM	1103	N	LEU	A	394	34.534	24.465	22.303	1.00	32.26	N
ATOM	1104	CA	LEU	A	394	34.436	23.653	21.121	1.00	31.95	C
ATOM	1105	CB	LEU	A	394	33.304	24.091	20.195	1.00	32.22	C
ATOM	1106	CG	LEU	A	394	31.829	23.898	20.560	1.00	30.03	C
ATOM	1107	CD1	LEU	A	394	30.964	24.445	19.463	1.00	27.50	C
ATOM	1108	CD2	LEU	A	394	31.547	22.458	20.809	1.00	31.13	C
ATOM	1109	C	LEU	A	394	35.720	23.720	20.316	1.00	32.56	C
ATOM	1110	O	LEU	A	394	35.948	22.892	19.493	1.00	32.76	O
ATOM	1111	N	GLY	A	395	36.520	24.749	20.498	1.00	35.25	N
ATOM	1112	CA	GLY	A	395	37.717	24.928	19.696	1.00	36.37	C
ATOM	1113	C	GLY	A	395	37.426	25.284	18.243	1.00	37.83	C
ATOM	1114	O	GLY	A	395	38.249	24.980	17.367	1.00	38.76	O
ATOM	1115	N	CYS	A	396	36.300	25.969	17.988	1.00	38.87	N
ATOM	1116	CA	CYS	A	396	35.877	26.363	16.626	1.00	39.61	C
ATOM	1117	CB	CYS	A	396	34.603	25.638	16.231	1.00	40.04	C
ATOM	1118	SG	CYS	A	396	34.493	23.892	16.532	1.00	47.12	S
ATOM	1119	C	CYS	A	396	35.483	27.836	16.522	1.00	38.76	C
ATOM	1120	O	CYS	A	396	34.364	28.140	16.063	1.00	37.44	O

ATOM	1121	N	GLU	A	397	36.359	28.747	16.928	1.00	38.45	N
ATOM	1122	CA	GLU	A	397	35.995	30.158	16.905	1.00	39.15	C
ATOM	1123	CB	GLU	A	397	37.123	31.064	17.392	1.00	39.98	C
ATOM	1124	CG	GLU	A	397	37.786	30.611	18.702	1.00	45.20	C
ATOM	1125	CD	GLU	A	397	37.249	31.254	19.991	1.00	51.31	C
ATOM	1126	OE1	GLU	A	397	36.045	31.041	20.323	1.00	55.26	O
ATOM	1127	OE2	GLU	A	397	38.046	31.920	20.717	1.00	53.17	O
ATOM	1128	C	GLU	A	397	35.487	30.605	15.520	1.00	37.80	C
ATOM	1129	O	GLU	A	397	34.511	31.296	15.465	1.00	37.56	O
ATOM	1130	N	ASP	A	398	36.118	30.197	14.423	1.00	37.26	N
ATOM	1131	CA	ASP	A	398	35.685	30.640	13.091	1.00	37.80	C
ATOM	1132	CB	ASP	A	398	36.695	30.253	12.000	1.00	39.29	C
ATOM	1133	CG	ASP	A	398	38.008	31.019	12.097	1.00	42.86	C
ATOM	1134	OD1	ASP	A	398	38.097	32.024	12.844	1.00	48.94	O
ATOM	1135	OD2	ASP	A	398	39.018	30.660	11.450	1.00	47.39	O
ATOM	1136	C	ASP	A	398	34.305	30.103	12.676	1.00	35.53	C
ATOM	1137	O	ASP	A	398	33.472	30.848	12.182	1.00	35.67	O
ATOM	1138	N	PHE	A	399	34.075	28.814	12.852	1.00	33.02	N
ATOM	1139	CA	PHE	A	399	32.755	28.264	12.574	1.00	31.62	C
ATOM	1140	CB	PHE	A	399	32.757	26.754	12.735	1.00	31.05	C
ATOM	1141	CG	PHE	A	399	31.399	26.151	12.729	1.00	30.78	C
ATOM	1142	CD1	PHE	A	399	30.702	26.027	11.567	1.00	30.86	C
ATOM	1143	CE1	PHE	A	399	29.437	25.502	11.561	1.00	31.41	C
ATOM	1144	CZ	PHE	A	399	28.856	25.092	12.742	1.00	31.17	C
ATOM	1145	CE2	PHE	A	399	29.526	25.243	13.905	1.00	30.20	C
ATOM	1146	CD2	PHE	A	399	30.797	25.777	13.906	1.00	29.57	C
ATOM	1147	C	PHE	A	399	31.665	28.932	13.466	1.00	30.38	C
ATOM	1148	O	PHE	A	399	30.567	29.240	13.014	1.00	30.06	O
ATOM	1149	N	ILE	A	400	31.975	29.187	14.718	1.00	29.09	N
ATOM	1150	CA	ILE	A	400	30.988	29.793	15.584	1.00	28.21	C
ATOM	1151	CB	ILE	A	400	31.453	29.709	17.022	1.00	27.49	C
ATOM	1152	CG1	ILE	A	400	31.426	28.255	17.501	1.00	28.01	C
ATOM	1153	CD1	ILE	A	400	30.013	27.629	17.525	1.00	27.35	C
ATOM	1154	CG2	ILE	A	400	30.557	30.501	17.930	1.00	28.61	C
ATOM	1155	C	ILE	A	400	30.717	31.213	15.132	1.00	28.30	C
ATOM	1156	O	ILE	A	400	29.538	31.652	15.105	1.00	27.29	O
ATOM	1157	N	SER	A	401	31.774	31.949	14.758	1.00	27.64	N
ATOM	1158	CA	SER	A	401	31.552	33.329	14.298	1.00	28.85	C
ATOM	1159	CB	SER	A	401	32.850	34.152	14.224	1.00	28.93	C
ATOM	1160	OG	SER	A	401	33.622	33.761	13.129	1.00	35.10	O
ATOM	1161	C	SER	A	401	30.736	33.397	12.997	1.00	27.77	C
ATOM	1162	O	SER	A	401	29.938	34.283	12.818	1.00	28.99	O
ATOM	1163	N	PHE	A	402	30.910	32.423	12.133	1.00	27.14	N
ATOM	1164	CA	PHE	A	402	30.144	32.276	10.923	1.00	27.41	C
ATOM	1165	CB	PHE	A	402	30.800	31.145	10.137	1.00	27.67	C
ATOM	1166	CG	PHE	A	402	30.303	30.940	8.733	1.00	30.03	C
ATOM	1167	CD1	PHE	A	402	29.486	31.840	8.091	1.00	31.94	C
ATOM	1168	CE1	PHE	A	402	29.061	31.618	6.813	1.00	30.13	C
ATOM	1169	CZ	PHE	A	402	29.438	30.512	6.124	1.00	30.57	C
ATOM	1170	CE2	PHE	A	402	30.266	29.595	6.712	1.00	33.09	C
ATOM	1171	CD2	PHE	A	402	30.704	29.815	8.030	1.00	34.00	C
ATOM	1172	C	PHE	A	402	28.657	31.992	11.290	1.00	26.84	C
ATOM	1173	O	PHE	A	402	27.733	32.571	10.717	1.00	25.94	O
ATOM	1174	N	VAL	A	403	28.416	31.141	12.280	1.00	26.02	N
ATOM	1175	CA	VAL	A	403	27.035	30.855	12.669	1.00	25.17	C
ATOM	1176	CB	VAL	A	403	26.967	29.787	13.797	1.00	24.18	C
ATOM	1177	CG1	VAL	A	403	25.606	29.750	14.394	1.00	25.35	C
ATOM	1178	CG2	VAL	A	403	27.294	28.446	13.255	1.00	24.23	C
ATOM	1179	C	VAL	A	403	26.339	32.131	13.158	1.00	24.80	C
ATOM	1180	O	VAL	A	403	25.194	32.422	12.831	1.00	24.70	O
ATOM	1181	N	PHE	A	404	27.011	32.868	13.998	1.00	24.99	N
ATOM	1182	CA	PHE	A	404	26.398	34.058	14.547	1.00	25.96	C
ATOM	1183	CB	PHE	A	404	27.212	34.579	15.719	1.00	26.02	C
ATOM	1184	CG	PHE	A	404	26.912	33.880	17.037	1.00	25.96	C
ATOM	1185	CD1	PHE	A	404	27.378	32.614	17.296	1.00	26.60	C
ATOM	1186	CE1	PHE	A	404	27.087	31.962	18.535	1.00	27.71	C

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ATOM	1187	CZ	PHE	A	404	26.358	32.572	19.475	1.00	26.31	C
ATOM	1188	CE2	PHE	A	404	25.881	33.846	19.230	1.00	29.49	C
ATOM	1189	CD2	PHE	A	404	26.178	34.501	18.010	1.00	28.52	C
ATOM	1190	C	PHE	A	404	26.232	35.121	13.488	1.00	26.66	C
ATOM	1191	O	PHE	A	404	25.278	35.891	13.515	1.00	27.41	O
ATOM	1192	N	GLU	A	405	27.151	35.166	12.537	1.00	27.79	N
ATOM	1193	CA	GLU	A	405	27.078	36.165	11.487	1.00	27.80	C
ATOM	1194	CB	GLU	A	405	28.339	36.163	10.623	1.00	28.35	C
ATOM	1195	CG	GLU	A	405	28.147	37.016	9.384	1.00	31.23	C
ATOM	1196	CD	GLU	A	405	29.446	37.528	8.769	1.00	35.82	C
ATOM	1197	OE1	GLU	A	405	30.552	37.009	9.096	1.00	37.08	O
ATOM	1198	OE2	GLU	A	405	29.334	38.448	7.937	1.00	35.95	O
ATOM	1199	C	GLU	A	405	25.861	35.864	10.629	1.00	27.96	C
ATOM	1200	O	GLU	A	405	25.126	36.773	10.228	1.00	25.82	O
ATOM	1201	N	PHE	A	406	25.658	34.576	10.373	1.00	27.97	N
ATOM	1202	CA	PHE	A	406	24.508	34.148	9.629	1.00	29.23	C
ATOM	1203	CB	PHE	A	406	24.549	32.656	9.326	1.00	28.50	C
ATOM	1204	CG	PHE	A	406	23.459	32.229	8.434	1.00	29.33	C
ATOM	1205	CD1	PHE	A	406	23.588	32.396	7.058	1.00	31.26	C
ATOM	1206	CE1	PHE	A	406	22.574	32.049	6.214	1.00	29.99	C
ATOM	1207	CZ	PHE	A	406	21.389	31.531	6.737	1.00	30.86	C
ATOM	1208	CE2	PHE	A	406	21.253	31.340	8.104	1.00	30.00	C
ATOM	1209	CD2	PHE	A	406	22.277	31.698	8.949	1.00	27.04	C
ATOM	1210	C	PHE	A	406	23.204	34.511	10.367	1.00	30.08	C
ATOM	1211	O	PHE	A	406	22.238	34.936	9.746	1.00	29.57	O
ATOM	1212	N	GLY	A	407	23.186	34.337	11.681	1.00	31.28	N
ATOM	1213	CA	GLY	A	407	22.009	34.643	12.485	1.00	31.96	C
ATOM	1214	C	GLY	A	407	21.699	36.116	12.401	1.00	33.32	C
ATOM	1215	O	GLY	A	407	20.581	36.539	12.135	1.00	32.80	O
ATOM	1216	N	LYS	A	408	22.729	36.915	12.577	1.00	35.20	N
ATOM	1217	CA	LYS	A	408	22.586	38.344	12.430	1.00	36.71	C
ATOM	1218	CB	LYS	A	408	23.931	38.993	12.688	1.00	37.55	C
ATOM	1219	CG	LYS	A	408	23.845	40.473	12.958	1.00	40.89	C
ATOM	1220	CD	LYS	A	408	25.125	41.000	13.605	1.00	44.55	C
ATOM	1221	CE	LYS	A	408	25.143	40.758	15.121	1.00	46.16	C
ATOM	1222	NZ	LYS	A	408	26.310	41.466	15.786	1.00	47.26	N
ATOM	1223	C	LYS	A	408	22.090	38.756	11.033	1.00	37.33	C
ATOM	1224	O	LYS	A	408	21.233	39.637	10.881	1.00	37.08	O
ATOM	1225	N	SER	A	409	22.610	38.106	10.005	1.00	37.62	N
ATOM	1226	CA	SER	A	409	22.258	38.499	8.649	1.00	38.03	C
ATOM	1227	CB	SER	A	409	23.258	37.906	7.681	1.00	37.87	C
ATOM	1228	OG	SER	A	409	22.671	37.759	6.421	1.00	43.04	O
ATOM	1229	C	SER	A	409	20.816	38.139	8.273	1.00	37.59	C
ATOM	1230	O	SER	A	409	20.146	38.891	7.596	1.00	37.65	O
ATOM	1231	N	LEU	A	410	20.330	36.994	8.730	1.00	38.00	N
ATOM	1232	CA	LEU	A	410	18.944	36.599	8.476	1.00	38.06	C
ATOM	1233	CB	LEU	A	410	18.771	35.108	8.728	1.00	37.93	C
ATOM	1234	CG	LEU	A	410	17.711	34.363	7.930	1.00	39.48	C
ATOM	1235	CD1	LEU	A	410	17.866	34.566	6.431	1.00	40.64	C
ATOM	1236	CD2	LEU	A	410	17.795	32.873	8.280	1.00	39.84	C
ATOM	1237	C	LEU	A	410	17.969	37.447	9.323	1.00	37.89	C
ATOM	1238	O	LEU	A	410	16.907	37.826	8.859	1.00	36.02	O
ATOM	1239	N	CYS	A	411	18.344	37.745	10.558	1.00	39.15	N
ATOM	1240	CA	CYS	A	411	17.552	38.634	11.416	1.00	40.62	C
ATOM	1241	CB	CYS	A	411	18.243	38.819	12.753	1.00	41.09	C
ATOM	1242	SG	CYS	A	411	18.069	37.449	13.893	1.00	41.89	S
ATOM	1243	C	CYS	A	411	17.371	40.029	10.822	1.00	41.43	C
ATOM	1244	O	CYS	A	411	16.301	40.596	10.880	1.00	41.63	O
ATOM	1245	N	SER	A	412	18.433	40.579	10.253	1.00	42.39	N
ATOM	1246	CA	SER	A	412	18.381	41.897	9.641	1.00	43.17	C
ATOM	1247	CB	SER	A	412	19.756	42.278	9.067	1.00	42.83	C
ATOM	1248	OG	SER	A	412	19.897	41.811	7.730	1.00	43.89	O
ATOM	1249	C	SER	A	412	17.325	42.003	8.534	1.00	44.19	C
ATOM	1250	O	SER	A	412	17.030	43.119	8.072	1.00	45.40	O
ATOM	1251	N	MET	A	413	16.771	40.880	8.085	1.00	43.86	N
ATOM	1252	CA	MET	A	413	15.732	40.913	7.065	1.00	44.53	C

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ATOM	1253	CB	MET	A	413	15.874	39.740	6.102	1.00	44.68	C
ATOM	1254	CG	MET	A	413	17.179	39.724	5.375	1.00	45.77	C
ATOM	1255	SD	MET	A	413	17.293	38.227	4.484	1.00	52.29	S
ATOM	1256	CE	MET	A	413	19.021	38.123	4.084	1.00	52.15	C
ATOM	1257	C	MET	A	413	14.319	40.920	7.666	1.00	44.82	C
ATOM	1258	O	MET	A	413	13.354	41.154	6.948	1.00	45.27	O
ATOM	1259	N	HIS	A	414	14.207	40.686	8.969	1.00	44.42	N
ATOM	1260	CA	HIS	A	414	12.917	40.694	9.651	1.00	45.37	C
ATOM	1261	CB	HIS	A	414	12.369	42.124	9.831	1.00	46.54	C
ATOM	1262	CG	HIS	A	414	13.414	43.131	10.202	1.00	49.03	C
ATOM	1263	ND1	HIS	A	414	13.905	43.252	11.484	1.00	52.00	N
ATOM	1264	CE1	HIS	A	414	14.830	44.198	11.511	1.00	52.74	C
ATOM	1265	NE2	HIS	A	414	14.956	44.694	10.290	1.00	53.78	N
ATOM	1266	CD2	HIS	A	414	14.078	44.046	9.452	1.00	51.02	C
ATOM	1267	C	HIS	A	414	11.920	39.867	8.867	1.00	44.54	C
ATOM	1268	O	HIS	A	414	10.905	40.380	8.397	1.00	45.13	O
ATOM	1269	N	LEU	A	415	12.221	38.586	8.712	1.00	43.37	N
ATOM	1270	CA	LEU	A	415	11.345	37.696	7.992	1.00	42.05	C
ATOM	1271	CB	LEU	A	415	12.098	36.448	7.563	1.00	42.25	C
ATOM	1272	CG	LEU	A	415	13.274	36.739	6.635	1.00	42.37	C
ATOM	1273	CD1	LEU	A	415	14.213	35.584	6.615	1.00	43.50	C
ATOM	1274	CD2	LEU	A	415	12.736	37.013	5.254	1.00	42.77	C
ATOM	1275	C	LEU	A	415	10.200	37.311	8.889	1.00	41.21	C
ATOM	1276	O	LEU	A	415	10.379	37.116	10.073	1.00	40.43	O
ATOM	1277	N	THR	A	416	9.019	37.191	8.310	1.00	40.22	N
ATOM	1278	CA	THR	A	416	7.852	36.771	9.050	1.00	39.80	C
ATOM	1279	CB	THR	A	416	6.587	37.152	8.269	1.00	39.84	C
ATOM	1280	OG1	THR	A	416	6.623	36.538	6.978	1.00	39.74	O
ATOM	1281	CG2	THR	A	416	6.546	38.636	7.950	1.00	39.98	C
ATOM	1282	C	THR	A	416	7.890	35.270	9.203	1.00	39.01	C
ATOM	1283	O	THR	A	416	8.698	34.609	8.553	1.00	38.71	O
ATOM	1284	N	GLU	A	417	7.004	34.728	10.035	1.00	38.46	N
ATOM	1285	CA	GLU	A	417	6.925	33.289	10.241	1.00	38.70	C
ATOM	1286	CB	GLU	A	417	5.879	32.940	11.318	1.00	38.85	C
ATOM	1287	CG	GLU	A	417	6.350	33.068	12.768	1.00	41.11	C
ATOM	1288	CD	GLU	A	417	7.583	32.225	13.115	1.00	41.56	C
ATOM	1289	OE1	GLU	A	417	7.436	31.070	13.527	1.00	40.66	O
ATOM	1290	OE2	GLU	A	417	8.707	32.744	13.014	1.00	44.69	O
ATOM	1291	C	GLU	A	417	6.599	32.558	8.921	1.00	38.40	C
ATOM	1292	O	GLU	A	417	7.140	31.493	8.629	1.00	37.21	O
ATOM	1293	N	ASP	A	418	5.717	33.122	8.117	1.00	38.52	N
ATOM	1294	CA	ASP	A	418	5.382	32.489	6.845	1.00	39.36	C
ATOM	1295	CB	ASP	A	418	4.134	33.115	6.221	1.00	40.08	C
ATOM	1296	CG	ASP	A	418	2.858	32.783	7.007	1.00	44.36	C
ATOM	1297	OD1	ASP	A	418	2.931	31.961	7.953	1.00	50.10	O
ATOM	1298	OD2	ASP	A	418	1.736	33.282	6.742	1.00	48.86	O
ATOM	1299	C	ASP	A	418	6.540	32.531	5.865	1.00	38.10	C
ATOM	1300	O	ASP	A	418	6.712	31.634	5.057	1.00	37.14	O
ATOM	1301	N	GLU	A	419	7.311	33.602	5.925	1.00	37.67	N
ATOM	1302	CA	GLU	A	419	8.479	33.730	5.074	1.00	37.99	C
ATOM	1303	CB	GLU	A	419	9.062	35.165	5.163	1.00	38.22	C
ATOM	1304	CG	GLU	A	419	8.269	36.175	4.336	1.00	40.90	C
ATOM	1305	CD	GLU	A	419	8.530	37.629	4.682	1.00	41.76	C
ATOM	1306	OE1	GLU	A	419	9.193	37.895	5.685	1.00	43.26	O
ATOM	1307	OE2	GLU	A	419	8.059	38.512	3.938	1.00	45.04	O
ATOM	1308	C	GLU	A	419	9.519	32.657	5.459	1.00	36.84	C
ATOM	1309	O	GLU	A	419	10.106	32.012	4.590	1.00	36.16	O
ATOM	1310	N	ILE	A	420	9.708	32.453	6.760	1.00	35.93	N
ATOM	1311	CA	ILE	A	420	10.695	31.488	7.233	1.00	35.74	C
ATOM	1312	CB	ILE	A	420	10.899	31.607	8.740	1.00	36.17	C
ATOM	1313	CG1	ILE	A	420	11.712	32.873	9.008	1.00	38.07	C
ATOM	1314	CD1	ILE	A	420	11.838	33.228	10.464	1.00	39.66	C
ATOM	1315	CG2	ILE	A	420	11.617	30.377	9.287	1.00	36.15	C
ATOM	1316	C	ILE	A	420	10.311	30.085	6.856	1.00	34.34	C
ATOM	1317	O	ILE	A	420	11.156	29.282	6.517	1.00	33.17	O
ATOM	1318	N	ALA	A	421	9.013	29.813	6.914	1.00	33.91	N

ATOM	1319	CA	ALA	A	421
ATOM	1320	CB	ALA	A	421
ATOM	1321	C	ALA	A	421
ATOM	1322	O	ALA	A	421
ATOM	1323	N	LEU	A	422
ATOM	1324	CA	LEU	A	422
ATOM	1325	CB	LEU	A	422
ATOM	1326	CG	LEU	A	422
ATOM	1327	CD1	LEU	A	422
ATOM	1328	CD2	LEU	A	422
ATOM	1329	C	LEU	A	422
ATOM	1330	O	LEU	A	422
ATOM	1331	N	PHE	A	423
ATOM	1332	CA	PHE	A	423
ATOM	1333	CB	PHE	A	423
ATOM	1334	CG	PHE	A	423
ATOM	1335	CD1	PHE	A	423
ATOM	1336	CE1	PHE	A	423
ATOM	1337	CZ	PHE	A	423
ATOM	1338	CE2	PHE	A	423
ATOM	1339	CD2	PHE	A	423
ATOM	1340	C	PHE	A	423
ATOM	1341	O	PHE	A	423
ATOM	1342	N	SER	A	424
ATOM	1343	CA	SER	A	424
ATOM	1344	CB	SER	A	424
ATOM	1345	OG	SER	A	424
ATOM	1346	C	SER	A	424
ATOM	1347	O	SER	A	424
ATOM	1348	N	ALA	A	425
ATOM	1349	CA	ALA	A	425
ATOM	1350	CB	ALA	A	425
ATOM	1351	C	ALA	A	425
ATOM	1352	O	ALA	A	425
ATOM	1353	N	PHE	A	426
ATOM	1354	CA	PHE	A	426
ATOM	1355	CB	PHE	A	426
ATOM	1356	CG	PHE	A	426
ATOM	1357	CD1	PHE	A	426
ATOM	1358	CE1	PHE	A	426
ATOM	1359	CZ	PHE	A	426
ATOM	1360	CE2	PHE	A	426
ATOM	1361	CD2	PHE	A	426
ATOM	1362	C	PHE	A	426
ATOM	1363	O	PHE	A	426
ATOM	1364	N	VAL	A	427
ATOM	1365	CA	VAL	A	427
ATOM	1366	CB	VAL	A	427
ATOM	1367	CG1	VAL	A	427
ATOM	1368	CG2	VAL	A	427
ATOM	1369	C	VAL	A	427
ATOM	1370	O	VAL	A	427
ATOM	1371	N	LEU	A	428
ATOM	1372	CA	LEU	A	428
ATOM	1373	CB	LEU	A	428
ATOM	1374	CG	LEU	A	428
ATOM	1375	CD1	LEU	A	428
ATOM	1376	CD2	LEU	A	428
ATOM	1377	C	LEU	A	428
ATOM	1378	O	LEU	A	428
ATOM	1379	N	MET	A	429
ATOM	1380	CA	MET	A	429
ATOM	1381	CB	MET	A	429
ATOM	1382	CG	MET	A	429
ATOM	1383	SD	MET	A	429
ATOM	1384	CE	MET	A	429

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ATOM	1385	C	MET	A	429	14.293	20.979	-2.639	1.00	35.57	C
ATOM	1386	O	MET	A	429	13.772	21.578	-3.556	1.00	35.78	O
ATOM	1387	N	SER	A	430	15.602	20.813	-2.559	1.00	36.04	N
ATOM	1388	CA	SER	A	430	16.465	21.298	-3.608	1.00	37.23	C
ATOM	1389	CB	SER	A	430	17.782	21.792	-3.060	1.00	37.79	C
ATOM	1390	OG	SER	A	430	17.672	22.092	-1.698	1.00	40.76	O
ATOM	1391	C	SER	A	430	16.760	20.144	-4.507	1.00	37.02	C
ATOM	1392	O	SER	A	430	17.088	19.054	-4.034	1.00	37.47	O
ATOM	1393	N	ALA	A	431	16.683	20.375	-5.800	1.00	37.33	N
ATOM	1394	CA	ALA	A	431	16.869	19.301	-6.749	1.00	38.02	C
ATOM	1395	CB	ALA	A	431	16.086	19.581	-7.999	1.00	38.37	C
ATOM	1396	C	ALA	A	431	18.332	19.088	-7.071	1.00	39.47	C
ATOM	1397	O	ALA	A	431	18.675	18.155	-7.801	1.00	40.70	O
ATOM	1398	N	ASP	A	432	19.219	19.916	-6.528	1.00	40.30	N
ATOM	1399	CA	ASP	A	432	20.619	19.731	-6.853	1.00	41.30	C
ATOM	1400	CB	ASP	A	432	21.304	21.041	-7.201	1.00	42.25	C
ATOM	1401	CG	ASP	A	432	21.026	22.093	-6.217	1.00	45.95	C
ATOM	1402	OD1	ASP	A	432	21.919	22.947	-6.001	1.00	48.76	O
ATOM	1403	OD2	ASP	A	432	19.930	22.144	-5.610	1.00	53.78	O
ATOM	1404	C	ASP	A	432	21.425	18.985	-5.818	1.00	40.17	C
ATOM	1405	O	ASP	A	432	22.623	18.843	-5.968	1.00	42.18	O
ATOM	1406	N	ARG	A	433	20.810	18.440	-4.800	1.00	38.39	N
ATOM	1407	CA	ARG	A	433	21.597	17.625	-3.915	1.00	37.16	C
ATOM	1408	CB	ARG	A	433	20.744	17.081	-2.804	1.00	36.78	C
ATOM	1409	CG	ARG	A	433	19.976	18.117	-2.084	1.00	37.06	C
ATOM	1410	CD	ARG	A	433	20.810	19.149	-1.420	1.00	36.88	C
ATOM	1411	NE	ARG	A	433	19.938	19.958	-0.589	1.00	38.16	N
ATOM	1412	CZ	ARG	A	433	20.335	20.952	0.180	1.00	37.36	C
ATOM	1413	NH1	ARG	A	433	21.611	21.301	0.238	1.00	34.55	N
ATOM	1414	NH2	ARG	A	433	19.443	21.633	0.885	1.00	38.38	N
ATOM	1415	C	ARG	A	433	22.145	16.450	-4.731	1.00	37.08	C
ATOM	1416	O	ARG	A	433	21.441	15.925	-5.593	1.00	35.43	O
ATOM	1417	N	SER	A	434	23.370	16.022	-4.430	1.00	36.72	N
ATOM	1418	CA	SER	A	434	23.963	14.877	-5.105	1.00	36.76	C
ATOM	1419	CB	SER	A	434	25.390	14.603	-4.593	1.00	36.85	C
ATOM	1420	OG	SER	A	434	26.176	15.757	-4.604	1.00	38.46	O
ATOM	1421	C	SER	A	434	23.196	13.630	-4.782	1.00	36.80	C
ATOM	1422	O	SER	A	434	22.660	13.481	-3.670	1.00	35.82	O
ATOM	1423	N	TRP	A	435	23.206	12.720	-5.754	1.00	36.33	N
ATOM	1424	CA	TRP	A	435	22.706	11.376	-5.614	1.00	36.22	C
ATOM	1425	CB	TRP	A	435	23.314	10.715	-4.376	1.00	36.57	C
ATOM	1426	CG	TRP	A	435	24.778	10.979	-4.204	1.00	38.75	C
ATOM	1427	CD1	TRP	A	435	25.379	11.502	-3.115	1.00	40.89	C
ATOM	1428	NE1	TRP	A	435	26.733	11.585	-3.315	1.00	41.15	N
ATOM	1429	CE2	TRP	A	435	27.026	11.109	-4.560	1.00	39.69	C
ATOM	1430	CD2	TRP	A	435	25.825	10.717	-5.147	1.00	38.76	C
ATOM	1431	CE3	TRP	A	435	25.862	10.172	-6.425	1.00	40.76	C
ATOM	1432	CZ3	TRP	A	435	27.074	10.049	-7.063	1.00	41.43	C
ATOM	1433	CH2	TRP	A	435	28.250	10.450	-6.451	1.00	41.35	C
ATOM	1434	CZ2	TRP	A	435	28.249	10.976	-5.195	1.00	41.84	C
ATOM	1435	C	TRP	A	435	21.193	11.264	-5.575	1.00	36.43	C
ATOM	1436	O	TRP	A	435	20.674	10.269	-5.110	1.00	35.92	O
ATOM	1437	N	LEU	A	436	20.483	12.272	-6.048	1.00	37.43	N
ATOM	1438	CA	LEU	A	436	19.013	12.185	-6.139	1.00	38.64	C
ATOM	1439	CB	LEU	A	436	18.419	13.585	-6.194	1.00	38.27	C
ATOM	1440	CG	LEU	A	436	18.387	14.376	-4.902	1.00	37.94	C
ATOM	1441	CD1	LEU	A	436	17.844	15.752	-5.190	1.00	38.90	C
ATOM	1442	CD2	LEU	A	436	17.547	13.667	-3.885	1.00	37.76	C
ATOM	1443	C	LEU	A	436	18.531	11.436	-7.394	1.00	40.22	C
ATOM	1444	O	LEU	A	436	19.022	11.691	-8.497	1.00	40.43	O
ATOM	1445	N	GLN	A	437	17.542	10.562	-7.241	1.00	42.27	N
ATOM	1446	CA	GLN	A	437	16.981	9.825	-8.370	1.00	43.95	C
ATOM	1447	CB	GLN	A	437	16.334	8.537	-7.896	1.00	44.38	C
ATOM	1448	CG	GLN	A	437	17.247	7.710	-7.059	1.00	46.96	C
ATOM	1449	CD	GLN	A	437	16.647	6.389	-6.653	1.00	50.03	C
ATOM	1450	OE1	GLN	A	437	15.546	6.043	-7.084	1.00	54.83	O

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ATOM	1451	NE2	GLN	A	437	17.370	5.640	-5.826	1.00	50.03	N
ATOM	1452	C	GLN	A	437	15.958	10.644	-9.136	1.00	44.68	C
ATOM	1453	O	GLN	A	437	16.051	10.788	-10.346	1.00	45.04	O
ATOM	1454	N	GLU	A	438	15.000	11.221	-8.433	1.00	45.84	N
ATOM	1455	CA	GLU	A	438	13.933	11.977	-9.093	1.00	46.74	C
ATOM	1456	CB	GLU	A	438	12.628	11.716	-8.360	1.00	47.49	C
ATOM	1457	CG	GLU	A	438	12.433	10.254	-8.005	1.00	49.80	C
ATOM	1458	CD	GLU	A	438	11.318	10.066	-7.011	1.00	54.24	C
ATOM	1459	OE1	GLU	A	438	10.145	10.256	-7.410	1.00	55.09	O
ATOM	1460	OE2	GLU	A	438	11.625	9.744	-5.832	1.00	58.98	O
ATOM	1461	C	GLU	A	438	14.169	13.475	-9.154	1.00	46.63	C
ATOM	1462	O	GLU	A	438	13.399	14.242	-8.586	1.00	47.40	O
ATOM	1463	N	LYS	A	439	15.192	13.897	-9.887	1.00	46.50	N
ATOM	1464	CA	LYS	A	439	15.535	15.311	-9.995	1.00	45.87	C
ATOM	1465	CB	LYS	A	439	16.834	15.521	-10.794	1.00	46.05	C
ATOM	1466	CG	LYS	A	439	18.096	14.931	-10.113	1.00	48.48	C
ATOM	1467	CD	LYS	A	439	19.417	15.775	-10.247	1.00	51.35	C
ATOM	1468	CE	LYS	A	439	20.205	15.702	-8.875	1.00	54.04	C
ATOM	1469	NZ	LYS	A	439	21.624	16.236	-8.775	1.00	53.95	N
ATOM	1470	C	LYS	A	439	14.405	16.129	-10.609	1.00	45.17	C
ATOM	1471	O	LYS	A	439	14.149	17.248	-10.179	1.00	44.73	O
ATOM	1472	N	VAL	A	440	13.723	15.582	-11.607	1.00	44.46	N
ATOM	1473	CA	VAL	A	440	12.665	16.324	-12.279	1.00	43.79	C
ATOM	1474	CB	VAL	A	440	12.234	15.633	-13.601	1.00	44.85	C
ATOM	1475	CG1	VAL	A	440	10.895	16.199	-14.096	1.00	43.93	C
ATOM	1476	CG2	VAL	A	440	13.359	15.762	-14.686	1.00	44.89	C
ATOM	1477	C	VAL	A	440	11.437	16.574	-11.385	1.00	42.76	C
ATOM	1478	O	VAL	A	440	10.908	17.667	-11.371	1.00	42.48	O
ATOM	1479	N	LYS	A	441	10.981	15.582	-10.638	1.00	42.10	N
ATOM	1480	CA	LYS	A	441	9.842	15.811	-9.737	1.00	42.12	C
ATOM	1481	CB	LYS	A	441	9.337	14.469	-9.167	1.00	42.37	C
ATOM	1482	CG	LYS	A	441	8.268	14.551	-8.058	1.00	44.18	C
ATOM	1483	CD	LYS	A	441	7.770	13.145	-7.635	1.00	46.69	C
ATOM	1484	CE	LYS	A	441	7.415	13.029	-6.135	1.00	48.06	C
ATOM	1485	NZ	LYS	A	441	6.374	13.988	-5.640	1.00	50.40	N
ATOM	1486	C	LYS	A	441	10.222	16.812	-8.621	1.00	41.30	C
ATOM	1487	O	LYS	A	441	9.493	17.751	-8.337	1.00	41.41	O
ATOM	1488	N	ILE	A	442	11.384	16.639	-8.016	1.00	40.14	N
ATOM	1489	CA	ILE	A	442	11.792	17.530	-6.947	1.00	39.47	C
ATOM	1490	CB	ILE	A	442	13.092	17.036	-6.347	1.00	39.22	C
ATOM	1491	CG1	ILE	A	442	12.817	15.709	-5.642	1.00	37.84	C
ATOM	1492	CD1	ILE	A	442	14.038	14.971	-5.155	1.00	36.84	C
ATOM	1493	CG2	ILE	A	442	13.694	18.109	-5.421	1.00	38.41	C
ATOM	1494	C	ILE	A	442	11.924	18.939	-7.475	1.00	40.04	C
ATOM	1495	O	ILE	A	442	11.519	19.907	-6.828	1.00	39.89	O
ATOM	1496	N	GLU	A	443	12.474	19.068	-8.671	1.00	40.56	N
ATOM	1497	CA	GLU	A	443	12.583	20.380	-9.305	1.00	41.62	C
ATOM	1498	CB	GLU	A	443	13.325	20.252	-10.625	1.00	42.43	C
ATOM	1499	CG	GLU	A	443	13.473	21.556	-11.384	1.00	46.01	C
ATOM	1500	CD	GLU	A	443	14.586	22.409	-10.832	1.00	52.43	C
ATOM	1501	OE1	GLU	A	443	15.520	21.840	-10.224	1.00	58.50	O
ATOM	1502	OE2	GLU	A	443	14.540	23.649	-10.991	1.00	56.77	O
ATOM	1503	C	GLU	A	443	11.221	21.041	-9.531	1.00	41.19	C
ATOM	1504	O	GLU	A	443	11.051	22.217	-9.257	1.00	41.75	O
ATOM	1505	N	LYS	A	444	10.241	20.309	-10.027	1.00	41.34	N
ATOM	1506	CA	LYS	A	444	8.918	20.906	-10.222	1.00	41.91	C
ATOM	1507	CB	LYS	A	444	7.954	19.921	-10.887	1.00	42.50	C
ATOM	1508	CG	LYS	A	444	8.359	19.402	-12.287	1.00	46.11	C
ATOM	1509	CD	LYS	A	444	8.622	20.539	-13.249	1.00	50.76	C
ATOM	1510	CE	LYS	A	444	9.166	20.064	-14.593	1.00	53.57	C
ATOM	1511	NZ	LYS	A	444	10.041	21.141	-15.193	1.00	55.91	N
ATOM	1512	C	LYS	A	444	8.333	21.367	-8.869	1.00	41.11	C
ATOM	1513	O	LYS	A	444	7.669	22.385	-8.787	1.00	40.91	O
ATOM	1514	N	LEU	A	445	8.564	20.599	-7.811	1.00	40.57	N
ATOM	1515	CA	LEU	A	445	8.100	20.993	-6.475	1.00	40.29	C
ATOM	1516	CB	LEU	A	445	8.291	19.823	-5.510	1.00	40.73	C



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ATOM	1517	CG	LEU	A	445	7.471	18.577	-5.846	1.00	43.76	C
ATOM	1518	CD1	LEU	A	445	8.070	17.339	-5.224	1.00	46.83	C
ATOM	1519	CD2	LEU	A	445	6.006	18.699	-5.405	1.00	45.67	C
ATOM	1520	C	LEU	A	445	8.802	22.264	-5.932	1.00	39.05	C
ATOM	1521	O	LEU	A	445	8.162	23.148	-5.355	1.00	38.44	O
ATOM	1522	N	GLN	A	446	10.113	22.379	-6.131	1.00	37.84	N
ATOM	1523	CA	GLN	A	446	10.804	23.553	-5.630	1.00	37.19	C
ATOM	1524	CB	GLN	A	446	12.322	23.443	-5.770	1.00	36.98	C
ATOM	1525	CG	GLN	A	446	13.058	24.617	-5.128	1.00	38.75	C
ATOM	1526	CD	GLN	A	446	14.563	24.588	-5.312	1.00	40.58	C
ATOM	1527	OE1	GLN	A	446	15.065	24.583	-6.428	1.00	42.73	O
ATOM	1528	NE2	GLN	A	446	15.284	24.599	-4.206	1.00	41.51	N
ATOM	1529	C	GLN	A	446	10.312	24.808	-6.332	1.00	36.39	C
ATOM	1530	O	GLN	A	446	10.218	25.880	-5.715	1.00	35.15	O
ATOM	1531	N	GLN	A	447	10.037	24.680	-7.626	1.00	36.58	N
ATOM	1532	CA	GLN	A	447	9.547	25.810	-8.415	1.00	37.09	C
ATOM	1533	CB	GLN	A	447	9.316	25.428	-9.872	1.00	37.88	C
ATOM	1534	CG	GLN	A	447	10.545	25.058	-10.659	1.00	42.37	C
ATOM	1535	CD	GLN	A	447	10.176	24.683	-12.104	1.00	49.26	C
ATOM	1536	OE1	GLN	A	447	9.144	25.147	-12.634	1.00	53.32	O
ATOM	1537	NE2	GLN	A	447	10.993	23.831	-12.729	1.00	52.11	N
ATOM	1538	C	GLN	A	447	8.231	26.343	-7.845	1.00	35.60	C
ATOM	1539	O	GLN	A	447	8.075	27.518	-7.726	1.00	33.62	O
ATOM	1540	N	LYS	A	448	7.305	25.461	-7.508	1.00	35.56	N
ATOM	1541	CA	LYS	A	448	6.055	25.897	-6.903	1.00	36.26	C
ATOM	1542	CB	LYS	A	448	5.125	24.707	-6.684	1.00	36.75	C
ATOM	1543	CG	LYS	A	448	4.434	24.265	-7.968	1.00	41.05	C
ATOM	1544	CD	LYS	A	448	3.642	22.962	-7.752	1.00	45.62	C
ATOM	1545	CE	LYS	A	448	2.734	22.623	-8.941	1.00	47.75	C
ATOM	1546	NZ	LYS	A	448	1.655	21.655	-8.507	1.00	51.38	N
ATOM	1547	C	LYS	A	448	6.304	26.615	-5.584	1.00	35.43	C
ATOM	1548	O	LYS	A	448	5.762	27.697	-5.345	1.00	34.04	O
ATOM	1549	N	ILE	A	449	7.118	25.997	-4.720	1.00	35.23	N
ATOM	1550	CA	ILE	A	449	7.422	26.574	-3.428	1.00	35.08	C
ATOM	1551	CB	ILE	A	449	8.400	25.663	-2.647	1.00	35.31	C
ATOM	1552	CG1	ILE	A	449	7.662	24.412	-2.135	1.00	34.62	C
ATOM	1553	CD1	ILE	A	449	8.565	23.272	-1.666	1.00	35.68	C
ATOM	1554	CG2	ILE	A	449	9.036	26.439	-1.508	1.00	34.70	C
ATOM	1555	C	ILE	A	449	8.009	27.950	-3.648	1.00	35.67	C
ATOM	1556	O	ILE	A	449	7.663	28.891	-2.954	1.00	36.39	O
ATOM	1557	N	GLN	A	450	8.863	28.092	-4.648	1.00	36.15	N
ATOM	1558	CA	GLN	A	450	9.491	29.383	-4.898	1.00	37.22	C
ATOM	1559	CB	GLN	A	450	10.624	29.245	-5.929	1.00	37.71	C
ATOM	1560	CG	GLN	A	450	11.440	30.525	-6.143	1.00	39.93	C
ATOM	1561	CD	GLN	A	450	12.459	30.381	-7.271	1.00	44.24	C
ATOM	1562	OE1	GLN	A	450	13.107	29.339	-7.409	1.00	46.56	O
ATOM	1563	NE2	GLN	A	450	12.603	31.421	-8.071	1.00	46.99	N
ATOM	1564	C	GLN	A	450	8.497	30.453	-5.351	1.00	37.23	C
ATOM	1565	O	GLN	A	450	8.668	31.629	-5.033	1.00	36.57	O
ATOM	1566	N	LEU	A	451	7.460	30.067	-6.095	1.00	37.47	N
ATOM	1567	CA	LEU	A	451	6.491	31.055	-6.548	1.00	38.17	C
ATOM	1568	CB	LEU	A	451	5.602	30.496	-7.658	1.00	39.23	C
ATOM	1569	CG	LEU	A	451	6.299	30.228	-8.992	1.00	40.16	C
ATOM	1570	CD1	LEU	A	451	5.417	29.356	-9.874	1.00	42.60	C
ATOM	1571	CD2	LEU	A	451	6.671	31.543	-9.709	1.00	40.87	C
ATOM	1572	C	LEU	A	451	5.675	31.479	-5.350	1.00	38.38	C
ATOM	1573	O	LEU	A	451	5.328	32.670	-5.177	1.00	37.56	O
ATOM	1574	N	ALA	A	452	5.396	30.500	-4.499	1.00	38.51	N
ATOM	1575	CA	ALA	A	452	4.683	30.763	-3.261	1.00	39.16	C
ATOM	1576	CB	ALA	A	452	4.352	29.452	-2.566	1.00	39.25	C
ATOM	1577	C	ALA	A	452	5.492	31.668	-2.335	1.00	39.16	C
ATOM	1578	O	ALA	A	452	4.960	32.541	-1.667	1.00	38.45	O
ATOM	1579	N	LEU	A	453	6.793	31.461	-2.302	1.00	39.99	N
ATOM	1580	CA	LEU	A	453	7.650	32.284	-1.454	1.00	40.16	C
ATOM	1581	CB	LEU	A	453	9.078	31.735	-1.455	1.00	39.61	C
ATOM	1582	CG	LEU	A	453	10.108	32.594	-0.724	1.00	38.75	C

ATOM	1583	CD1	LEU	A	453	9.785	32.702	0.737	1.00	37.68
ATOM	1584	CD2	LEU	A	453	11.487	31.994	-0.924	1.00	39.28
ATOM	1585	C	LEU	A	453	7.649	33.727	-1.936	1.00	41.01
ATOM	1586	O	LEU	A	453	7.559	34.652	-1.143	1.00	40.74
ATOM	1587	N	GLN	A	454	7.784	33.912	-3.245	1.00	43.21
ATOM	1588	CA	GLN	A	454	7.778	35.242	-3.857	1.00	44.37
ATOM	1589	CB	GLN	A	454	8.018	35.097	-5.353	1.00	44.93
ATOM	1590	CG	GLN	A	454	8.139	36.413	-6.092	1.00	47.00
ATOM	1591	CD	GLN	A	454	8.484	36.232	-7.549	1.00	50.13
ATOM	1592	OE1	GLN	A	454	7.937	35.355	-8.224	1.00	51.04
ATOM	1593	NE2	GLN	A	454	9.397	37.062	-8.044	1.00	52.53
ATOM	1594	C	GLN	A	454	6.438	35.937	-3.580	1.00	45.15
ATOM	1595	O	GLN	A	454	6.385	37.105	-3.193	1.00	45.17
ATOM	1596	N	HIS	A	455	5.363	35.186	-3.735	1.00	46.23
ATOM	1597	CA	HIS	A	455	4.029	35.654	-3.418	1.00	47.70
ATOM	1598	CB	HIS	A	455	3.064	34.479	-3.557	1.00	47.88
ATOM	1599	CG	HIS	A	455	1.659	34.782	-3.164	1.00	50.63
ATOM	1600	ND1	HIS	A	455	0.939	35.826	-3.706	1.00	52.70
ATOM	1601	CE1	HIS	A	455	-0.272	35.843	-3.172	1.00	53.57
ATOM	1602	NE2	HIS	A	455	-0.363	34.844	-2.309	1.00	53.78
ATOM	1603	CD2	HIS	A	455	0.833	34.167	-2.283	1.00	52.74
ATOM	1604	C	HIS	A	455	3.974	36.276	-2.018	1.00	48.21
ATOM	1605	O	HIS	A	455	3.561	37.425	-1.852	1.00	48.61
ATOM	1606	N	VAL	A	456	4.436	35.544	-1.017	1.00	48.96
ATOM	1607	CA	VAL	A	456	4.409	36.035	0.369	1.00	49.83
ATOM	1608	CB	VAL	A	456	4.656	34.884	1.353	1.00	49.91
ATOM	1609	CG1	VAL	A	456	4.882	35.394	2.759	1.00	50.35
ATOM	1610	CG2	VAL	A	456	3.498	33.899	1.325	1.00	50.07
ATOM	1611	C	VAL	A	456	5.437	37.101	0.684	1.00	50.39
ATOM	1612	O	VAL	A	456	5.262	37.865	1.625	1.00	50.47
ATOM	1613	N	LEU	A	457	6.529	37.119	-0.062	1.00	51.74
ATOM	1614	CA	LEU	A	457	7.538	38.140	0.143	1.00	53.31
ATOM	1615	CB	LEU	A	457	8.801	37.829	-0.648	1.00	53.04
ATOM	1616	CG	LEU	A	457	9.664	36.711	-0.065	1.00	52.30
ATOM	1617	CD1	LEU	A	457	10.705	36.350	-1.081	1.00	51.56
ATOM	1618	CD2	LEU	A	457	10.296	37.172	1.254	1.00	50.93
ATOM	1619	C	LEU	A	457	6.979	39.480	-0.294	1.00	55.43
ATOM	1620	O	LEU	A	457	7.071	40.456	0.437	1.00	54.68
ATOM	1621	N	GLN	A	458	6.372	39.516	-1.480	1.00	58.58
ATOM	1622	CA	GLN	A	458	5.836	40.764	-2.020	1.00	61.31
ATOM	1623	CB	GLN	A	458	5.596	40.661	-3.538	1.00	61.66
ATOM	1624	CG	GLN	A	458	4.556	39.646	-4.008	1.00	63.40
ATOM	1625	CD	GLN	A	458	4.816	39.189	-5.449	1.00	65.86
ATOM	1626	OE1	GLN	A	458	5.793	39.622	-6.069	1.00	67.19
ATOM	1627	NE2	GLN	A	458	3.949	38.313	-5.978	1.00	66.76
ATOM	1628	C	GLN	A	458	4.591	41.256	-1.265	1.00	63.26
ATOM	1629	O	GLN	A	458	4.268	42.434	-1.282	1.00	63.33
ATOM	1630	N	LYS	A	459	3.929	40.359	-0.560	1.00	65.71
ATOM	1631	CA	LYS	A	459	2.770	40.732	0.228	1.00	67.66
ATOM	1632	CB	LYS	A	459	2.241	39.477	0.894	1.00	67.68
ATOM	1633	CG	LYS	A	459	1.061	39.617	1.825	1.00	67.62
ATOM	1634	CD	LYS	A	459	0.638	38.243	2.332	1.00	67.67
ATOM	1635	CE	LYS	A	459	-0.042	37.427	1.241	1.00	67.92
ATOM	1636	NZ	LYS	A	459	-0.160	35.983	1.597	1.00	68.58
ATOM	1637	C	LYS	A	459	3.116	41.776	1.290	1.00	69.97
ATOM	1638	O	LYS	A	459	2.285	42.618	1.648	1.00	70.29
ATOM	1639	N	ASN	A	460	4.361	41.747	1.755	1.00	72.42
ATOM	1640	CA	ASN	A	460	4.802	42.571	2.871	1.00	74.25
ATOM	1641	CB	ASN	A	460	5.508	41.681	3.896	1.00	74.44
ATOM	1642	CG	ASN	A	460	4.624	40.534	4.390	1.00	74.77
ATOM	1643	OD1	ASN	A	460	3.556	40.762	4.964	1.00	74.61
ATOM	1644	ND2	ASN	A	460	5.071	39.292	4.165	1.00	74.61
ATOM	1645	C	ASN	A	460	5.731	43.721	2.501	1.00	76.15
ATOM	1646	O	ASN	A	460	5.676	44.785	3.123	1.00	76.33
ATOM	1647	N	HIS	A	461	6.582	43.529	1.496	1.00	78.30
ATOM	1648	CA	HIS	A	461	7.564	44.550	1.141	1.00	79.89

ATOM	1649	CB	HIS	A	461	8.846	44.307	1.932	1.00	80.20
ATOM	1650	CG	HIS	A	461	8.629	44.208	3.407	1.00	81.84
ATOM	1651	ND1	HIS	A	461	8.597	45.312	4.234	1.00	84.02
ATOM	1652	CE1	HIS	A	461	8.377	44.919	5.478	1.00	84.23
ATOM	1653	NE2	HIS	A	461	8.253	43.603	5.484	1.00	83.90
ATOM	1654	CD2	HIS	A	461	8.406	43.135	4.201	1.00	83.33
ATOM	1655	C	HIS	A	461	7.907	44.600	-0.344	1.00	80.88
ATOM	1656	O	HIS	A	461	9.067	44.431	-0.721	1.00	80.77
ATOM	1657	N	ARG	A	462	6.912	44.841	-1.191	1.00	82.27
ATOM	1658	CA	ARG	A	462	7.194	45.051	-2.605	1.00	83.28
ATOM	1659	CB	ARG	A	462	5.903	45.330	-3.393	1.00	83.78
ATOM	1660	CG	ARG	A	462	5.303	44.070	-4.042	1.00	85.00
ATOM	1661	CD	ARG	A	462	3.898	44.230	-4.665	1.00	86.49
ATOM	1662	NE	ARG	A	462	3.505	43.033	-5.417	1.00	87.52
ATOM	1663	CZ	ARG	A	462	2.281	42.778	-5.865	1.00	88.16
ATOM	1664	NH1	ARG	A	462	1.283	43.636	-5.655	1.00	88.54
ATOM	1665	NH2	ARG	A	462	2.056	41.653	-6.532	1.00	87.86
ATOM	1666	C	ARG	A	462	8.191	46.222	-2.687	1.00	83.63
ATOM	1667	O	ARG	A	462	8.541	46.699	-3.770	1.00	83.73
ATOM	1668	N	GLU	A	463	8.649	46.649	-1.506	1.00	83.89
ATOM	1669	CA	GLU	A	463	9.624	47.723	-1.335	1.00	83.96
ATOM	1670	CB	GLU	A	463	9.847	47.970	0.156	1.00	84.16
ATOM	1671	CG	GLU	A	463	10.746	46.939	0.821	1.00	84.97
ATOM	1672	CD	GLU	A	463	10.741	47.071	2.326	1.00	85.96
ATOM	1673	OE1	GLU	A	463	10.286	48.126	2.808	1.00	87.00
ATOM	1674	OE2	GLU	A	463	11.182	46.126	3.020	1.00	86.69
ATOM	1675	C	GLU	A	463	10.980	47.413	-1.965	1.00	83.47
ATOM	1676	O	GLU	A	463	11.752	48.325	-2.276	1.00	83.54
ATOM	1677	N	ASP	A	464	11.274	46.125	-2.115	1.00	82.69
ATOM	1678	CA	ASP	A	464	12.532	45.673	-2.691	1.00	82.00
ATOM	1679	CB	ASP	A	464	13.576	45.440	-1.582	1.00	82.03
ATOM	1680	CG	ASP	A	464	14.138	46.743	-1.000	1.00	82.58
ATOM	1681	OD1	ASP	A	464	13.981	47.814	-1.626	1.00	82.80
ATOM	1682	OD2	ASP	A	464	14.766	46.795	0.079	1.00	82.96
ATOM	1683	C	ASP	A	464	12.251	44.380	-3.467	1.00	81.10
ATOM	1684	O	ASP	A	464	11.103	44.121	-3.868	1.00	81.10
ATOM	1685	N	GLY	A	465	13.305	43.599	-3.701	1.00	79.69
ATOM	1686	CA	GLY	A	465	13.210	42.292	-4.339	1.00	78.42
ATOM	1687	C	GLY	A	465	14.125	41.358	-3.567	1.00	77.09
ATOM	1688	O	GLY	A	465	15.055	40.776	-4.128	1.00	76.83
ATOM	1689	N	ILE	A	466	13.839	41.229	-2.269	1.00	75.34
ATOM	1690	CA	ILE	A	466	14.687	40.507	-1.318	1.00	73.67
ATOM	1691	CB	ILE	A	466	14.195	40.728	0.123	1.00	73.83
ATOM	1692	CG1								

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ATOM	1715	CG	LYS	A	469	19.486	39.829	0.860	1.00	62.89	C
ATOM	1716	CD	LYS	A	469	19.256	41.310	1.276	1.00	64.52	C
ATOM	1717	CE	LYS	A	469	19.505	41.608	2.756	1.00	65.74	C
ATOM	1718	NZ	LYS	A	469	18.942	42.951	3.178	1.00	66.28	C
ATOM	1719	C	LYS	A	469	18.854	37.133	-0.355	1.00	59.69	O
ATOM	1720	O	LYS	A	469	19.766	36.645	0.317	1.00	59.53	N
ATOM	1721	N	LEU	A	470	17.627	36.633	-0.360	1.00	57.33	C
ATOM	1722	CA	LEU	A	470	17.292	35.439	0.387	1.00	56.01	C
ATOM	1723	CB	LEU	A	470	15.771	35.324	0.527	1.00	55.44	C
ATOM	1724	CG	LEU	A	470	15.242	34.622	1.770	1.00	54.97	C
ATOM	1725	CD1	LEU	A	470	15.881	35.167	3.018	1.00	54.08	C
ATOM	1726	CD2	LEU	A	470	13.721	34.701	1.859	1.00	56.05	C
ATOM	1727	C	LEU	A	470	17.861	34.213	-0.331	1.00	55.43	C
ATOM	1728	O	LEU	A	470	18.522	33.382	0.281	1.00	54.90	O
ATOM	1729	N	ILE	A	471	17.624	34.111	-1.635	1.00	54.68	N
ATOM	1730	CA	ILE	A	471	18.120	32.986	-2.412	1.00	54.43	C
ATOM	1731	CB	ILE	A	471	17.538	33.016	-3.836	1.00	54.76	C
ATOM	1732	CG1	ILE	A	471	16.097	32.526	-3.792	1.00	55.40	C
ATOM	1733	CD1	ILE	A	471	15.438	32.478	-5.119	1.00	56.34	C
ATOM	1734	CG2	ILE	A	471	18.372	32.144	-4.798	1.00	55.26	C
ATOM	1735	C	ILE	A	471	19.631	33.016	-2.433	1.00	53.73	C
ATOM	1736	O	ILE	A	471	20.281	31.996	-2.616	1.00	53.69	O
ATOM	1737	N	CYS	A	472	20.189	34.198	-2.239	1.00	52.86	N
ATOM	1738	CA	CYS	A	472	21.625	34.347	-2.120	1.00	52.63	C
ATOM	1739	CB	CYS	A	472	21.979	35.829	-1.990	1.00	52.92	C
ATOM	1740	SG	CYS	A	472	22.874	36.495	-3.399	1.00	58.34	S
ATOM	1741	C	CYS	A	472	22.157	33.604	-0.886	1.00	50.97	C
ATOM	1742	O	CYS	A	472	23.290	33.104	-0.901	1.00	50.65	O
ATOM	1743	N	LYS	A	473	21.348	33.555	0.179	1.00	48.54	N
ATOM	1744	CA	LYS	A	473	21.758	32.936	1.439	1.00	47.29	C
ATOM	1745	CB	LYS	A	473	20.754	33.227	2.562	1.00	47.39	C
ATOM	1746	CG	LYS	A	473	20.619	34.712	2.930	1.00	49.59	C
ATOM	1747	CD	LYS	A	473	21.832	35.243	3.708	1.00	52.10	C
ATOM	1748	CE	LYS	A	473	22.062	36.733	3.414	1.00	54.59	C
ATOM	1749	NZ	LYS	A	473	23.470	37.017	2.981	1.00	56.43	N
ATOM	1750	C	LYS	A	473	21.875	31.450	1.277	1.00	45.26	C
ATOM	1751	O	LYS	A	473	22.631	30.804	1.995	1.00	45.05	O
ATOM	1752	N	VAL	A	474	21.122	30.919	0.327	1.00	43.23	N
ATOM	1753	CA	VAL	A	474	21.136	29.518	0.102	1.00	42.19	C
ATOM	1754	CB	VAL	A	474	20.387	29.116	-1.145	1.00	42.59	C
ATOM	1755	CG1	VAL	A	474	20.645	27.663	-1.449	1.00	42.42	C
ATOM	1756	CG2	VAL	A	474	18.910	29.383	-0.957	1.00	42.39	C
ATOM	1757	C	VAL	A	474	22.546	29.055	-0.055	1.00	41.04	C
ATOM	1758	O	VAL	A	474	22.919	28.042	0.503	1.00	39.72	O
ATOM	1759	N	SER	A	475	23.345	29.780	-0.812	1.00	39.27	N
ATOM	1760	CA	SER	A	475	24.718	29.353	-0.979	1.00	38.63	C
ATOM	1761	CB	SER	A	475	25.402	30.157	-2.070	1.00	38.92	C
ATOM	1762	OG	SER	A	475	26.788	29.921	-2.029	1.00	40.43	O
ATOM	1763	C	SER	A	475	25.490	29.483	0.336	1.00	37.50	C
ATOM	1764	O	SER	A	475	26.430	28.759	0.576	1.00	36.17	O
ATOM	1765	N	THR	A	476	25.118	30.425	1.192	1.00	36.92	N
ATOM	1766	CA	THR	A	476	25.854	30.597	2.443	1.00	36.78	C
ATOM	1767	CB	THR	A	476	25.460	31.898	3.133	1.00	37.27	C
ATOM	1768	OG1	THR	A	476	25.293	32.946	2.166	1.00	39.90	O
ATOM	1769	CG2	THR	A	476	26.543	32.416	4.043	1.00	37.41	C
ATOM	1770	C	THR	A	476	25.588	29.423	3.378	1.00	36.02	C
ATOM	1771	O	THR	A	476	26.489	28.981	4.084	1.00	35.49	O
ATOM	1772	N	LEU	A	477	24.355	28.916	3.360	1.00	35.62	N
ATOM	1773	CA	LEU	A	477	23.939	27.801	4.200	1.00	35.50	C
ATOM	1774	CB	LEU	A	477	22.457	27.515	4.019	1.00	35.72	C
ATOM	1775	CG	LEU	A	477	21.480	28.292	4.875	1.00	35.56	C
ATOM	1776	CD1	LEU	A	477	20.057	28.141	4.321	1.00	36.36	C
ATOM	1777	CD2	LEU	A	477	21.584	27.800	6.279	1.00	33.36	C
ATOM	1778	C	LEU	A	477	24.670	26.538	3.890	1.00	35.75	C
ATOM	1779	O	LEU	A	477	24.966	25.754	4.792	1.00	35.71	O
ATOM	1780	N	ARG	A	478	24.941	26.311	2.610	1.00	35.96	N

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ATOM	1781	CA	ARG	A	478	25.659	25.124	2.183	1.00	36.68	C
ATOM	1782	CB	ARG	A	478	25.606	24.989	0.666	1.00	37.49	C
ATOM	1783	CG	ARG	A	478	24.216	24.645	0.185	1.00	39.62	C
ATOM	1784	CD	ARG	A	478	24.110	24.375	-1.293	1.00	41.13	C
ATOM	1785	NE	ARG	A	478	22.727	24.112	-1.658	1.00	42.25	N
ATOM	1786	CZ	ARG	A	478	22.342	23.503	-2.763	1.00	43.78	N
ATOM	1787	NH1	ARG	A	478	23.246	23.088	-3.641	1.00	45.06	N
ATOM	1788	NH2	ARG	A	478	21.045	23.312	-3.003	1.00	42.39	N
ATOM	1789	C	ARG	A	478	27.093	25.179	2.666	1.00	36.22	C
ATOM	1790	O	ARG	A	478	27.655	24.170	3.056	1.00	36.31	O
ATOM	1791	N	ALA	A	479	27.690	26.361	2.645	1.00	35.43	N
ATOM	1792	CA	ALA	A	479	29.045	26.502	3.144	1.00	34.83	C
ATOM	1793	CB	ALA	A	479	29.634	27.829	2.714	1.00	34.35	C
ATOM	1794	C	ALA	A	479	29.029	26.382	4.674	1.00	34.50	C
ATOM	1795	O	ALA	A	479	29.923	25.803	5.254	1.00	33.03	O
ATOM	1796	N	LEU	A	480	28.011	26.924	5.330	1.00	34.39	N
ATOM	1797	CA	LEU	A	480	27.931	26.756	6.768	1.00	35.19	C
ATOM	1798	CB	LEU	A	480	26.787	27.598	7.348	1.00	35.91	C
ATOM	1799	CG	LEU	A	480	26.747	27.805	8.845	1.00	35.84	C
ATOM	1800	CD1	LEU	A	480	28.051	28.355	9.382	1.00	37.04	C
ATOM	1801	CD2	LEU	A	480	25.590	28.734	9.189	1.00	36.87	C
ATOM	1802	C	LEU	A	480	27.787	25.276	7.138	1.00	35.48	C
ATOM	1803	O	LEU	A	480	28.525	24.768	7.999	1.00	36.43	O
ATOM	1804	N	CYS	A	481	26.886	24.557	6.482	1.00	34.90	N
ATOM	1805	CA	CYS	A	481	26.721	23.150	6.768	1.00	35.75	C
ATOM	1806	CB	CYS	A	481	25.408	22.617	6.151	1.00	35.51	C
ATOM	1807	SG	CYS	A	481	23.970	23.492	6.880	1.00	39.57	S
ATOM	1808	C	CYS	A	481	27.955	22.339	6.343	1.00	35.95	C
ATOM	1809	O	CYS	A	481	28.248	21.278	6.914	1.00	35.58	O
ATOM	1810	N	GLY	A	482	28.690	22.846	5.359	1.00	35.86	N
ATOM	1811	CA	GLY	A	482	29.909	22.197	4.922	1.00	35.86	C
ATOM	1812	C	GLY	A	482	30.978	22.309	5.983	1.00	35.56	C
ATOM	1813	O	GLY	A	482	31.689	21.375	6.268	1.00	35.07	O
ATOM	1814	N	ARG	A	483	31.111	23.464	6.587	1.00	36.33	N
ATOM	1815	CA	ARG	A	483	32.099	23.572	7.623	1.00	37.63	C
ATOM	1816	CB	ARG	A	483	32.250	25.000	8.046	1.00	38.73	C
ATOM	1817	CG	ARG	A	483	32.770	25.873	6.900	1.00	43.48	C
ATOM	1818	CD	ARG	A	483	34.089	26.567	7.220	1.00	48.75	C
ATOM	1819	NE	ARG	A	483	34.129	27.928	6.699	1.00	52.27	N
ATOM	1820	CZ	ARG	A	483	34.148	29.016	7.463	1.00	56.41	C
ATOM	1821	NH1	ARG	A	483	34.138	28.914	8.793	1.00	55.60	N
ATOM	1822	NH2	ARG	A	483	34.177	30.224	6.894	1.00	59.68	N
ATOM	1823	C	ARG	A	483	31.767	22.661	8.813	1.00	37.14	C
ATOM	1824	O	ARG	A	483	32.662	22.026	9.401	1.00	36.58	O
ATOM	1825	N	HIS	A	484	30.486	22.567	9.161	1.00	36.27	N
ATOM	1826	CA	HIS	A	484	30.119	21.712	10.270	1.00	35.26	C
ATOM	1827	CB	HIS	A	484	28.615	21.655	10.449	1.00	34.25	C
ATOM	1828	CG	HIS	A	484	28.161	20.599	11.394	1.00	31.44	C
ATOM	1829	ND1	HIS	A	484	27.481	19.481	10.975	1.00	26.89	N
ATOM	1830	CE1	HIS	A	484	27.178	18.740	12.032	1.00	29.68	C
ATOM	1831	NE2	HIS	A	484	27.689	19.307	13.111	1.00	26.36	N
ATOM	1832	CD2	HIS	A	484	28.293	20.484	12.740	1.00	29.62	C
ATOM	1833	C	HIS	A	484	30.656	20.333	10.013	1.00	36.35	C
ATOM	1834	O	HIS	A	484	31.264	19.740	10.893	1.00	35.93	O
ATOM	1835	N	THR	A	485	30.457	19.818	8.805	1.00	38.13	N
ATOM	1836	CA	THR	A	485	30.881	18.466	8.520	1.00	39.75	C
ATOM	1837	CB	THR	A	485	30.421	18.032	7.111	1.00	40.58	C
ATOM	1838	OG1	THR	A	485	29.011	17.726	7.102	1.00	42.13	O
ATOM	1839	CG2	THR	A	485	31.050	16.685	6.702	1.00	41.01	C
ATOM	1840	C	THR	A	485	32.404	18.340	8.663	1.00	40.64	C
ATOM	1841	O	THR	A	485	32.903	17.312	9.092	1.00	41.11	O
ATOM	1842	N	GLU	A	486	33.136	19.380	8.297	1.00	41.10	N
ATOM	1843	CA	GLU	A	486	34.583	19.329	8.343	1.00	41.77	C
ATOM	1844	CB	GLU	A	486	35.200	20.533	7.597	1.00	42.58	C
ATOM	1845	CG	GLU	A	486	35.297	20.311	6.080	1.00	45.90	C
ATOM	1846	CD	GLU	A	486	35.265	21.577	5.215	1.00	48.00	C

ATOM	1847	OE1	GLU	A	486	34.972	21.411	4.013	1.00	50.12
ATOM	1848	OE2	GLU	A	486	35.538	22.715	5.690	1.00	50.93
ATOM	1849	C	GLU	A	486	35.048	19.311	9.775	1.00	40.94
ATOM	1850	O	GLU	A	486	35.970	18.573	10.146	1.00	40.53
ATOM	1851	N	LYS	A	487	34.445	20.161	10.584	1.00	39.75
ATOM	1852	CA	LYS	A	487	34.828	20.215	11.976	1.00	38.97
ATOM	1853	CB	LYS	A	487	34.122	21.369	12.697	1.00	39.27
ATOM	1854	CG	LYS	A	487	34.760	22.719	12.395	1.00	42.48
ATOM	1855	CD	LYS	A	487	36.275	22.575	12.241	1.00	45.26
ATOM	1856	CE	LYS	A	487	36.953	23.908	12.119	1.00	47.44
ATOM	1857	NZ	LYS	A	487	37.048	24.550	13.468	1.00	50.31
ATOM	1858	C	LYS	A	487	34.509	18.896	12.637	1.00	38.04
ATOM	1859	O	LYS	A	487	35.306	18.390	13.405	1.00	37.61
ATOM	1860	N	LEU	A	488	33.354	18.329	12.317	1.00	37.23
ATOM	1861	CA	LEU	A	488	32.937	17.098	12.946	1.00	37.18
ATOM	1862	CB	LEU	A	488	31.502	16.755	12.561	1.00	36.30
ATOM	1863	CG	LEU	A	488	31.030	15.382	12.993	1.00	36.25
ATOM	1864	CD1	LEU	A	488	31.060	15.184	14.496	1.00	37.06
ATOM	1865	CD2	LEU	A	488	29.636	15.172	12.465	1.00	37.46
ATOM	1866	C	LEU	A	488	33.885	15.955	12.593	1.00	37.99
ATOM	1867	O	LEU	A	488	34.238	15.147	13.466	1.00	37.01
ATOM	1868	N	MET	A	489	34.263	15.851	11.317	1.00	38.60
ATOM	1869	CA	MET	A	489	35.240	14.828	10.932	1.00	40.07
ATOM	1870	CB	MET	A	489	35.412	14.694	9.409	1.00	40.81
ATOM	1871	CG	MET	A	489	34.178	14.171	8.704	1.00	44.15
ATOM	1872	SD	MET	A	489	33.194	12.913	9.641	1.00	54.88
ATOM	1873	CE	MET	A	489	33.908	11.239	9.132	1.00	55.79
ATOM	1874	C	MET	A	489	36.572	15.107	11.636	1.00	39.24
ATOM	1875	O	MET	A	489	37.216	14.197	12.086	1.00	38.99
ATOM	1876	N	ALA	A	490	36.960	16.356	11.813	1.00	39.22
ATOM	1877	CA	ALA	A	490	38.226	16.606	12.512	1.00	39.46
ATOM	1878	CB	ALA	A	490	38.623	18.062	12.412	1.00	38.63
ATOM	1879	C	ALA	A	490	38.152	16.166	13.997	1.00	40.06
ATOM	1880	O	ALA	A	490	39.131	15.669	14.568	1.00	40.68
ATOM	1881	N	PHE	A	491	36.979	16.351	14.602	1.00	39.40
ATOM	1882	CA	PHE	A	491	36.756	15.996	15.982	1.00	38.41
ATOM	1883	CB	PHE	A	491	35.449	16.640	16.482	1.00	37.82
ATOM	1884	CG	PHE	A	491	35.055	16.218	17.871	1.00	34.23
ATOM	1885	CD1	PHE	A	491	35.515	16.907	18.979	1.00	31.46
ATOM	1886	CE1	PHE	A	491	35.168	16.507	20.263	1.00	31.14
ATOM	1887	CZ	PHE	A	491	34.329	15.411	20.445	1.00	29.45
ATOM	1888	CE2	PHE	A	491	33.873	14.724	19.340	1.00	32.47
ATOM	1889	CD2	PHE	A	491	34.233	15.134	18.058	1.00	31.03
ATOM	1890	C	PHE	A	491	36.695	14.484	16.112	1.00	39.01
ATOM	1891	O	PHE	A	491	37.183	13.910	17.079	1.00	38.94
ATOM	1892	N	LYS	A	492	36.077	13.831	15.153	1.00	39.53
ATOM	1893	CA	LYS	A	492	35.941	12.401	15.226	1.00	40.55
ATOM	1894	CB	LYS	A	492	34.934	11.958	14.192	1.00	40.93
ATOM	1895	CG	LYS	A	492	34.730	10.473	14.114	1.00	42.40
ATOM	1896	CD	LYS	A	492	33.670	10.118	13.098	1.00	44.01
ATOM	1897	CE	LYS	A	492	33.493	8.628	12.999	1.00	44.96
ATOM	1898	NZ	LYS	A	492	32.414	8.271	12.044	1.00	47.85
ATOM	1899	C	LYS	A	492	37.283	11.668	15.031	1.00	41.46
ATOM	1900	O	LYS	A	492	37.425	10.516	15.389	1.00	41.69
ATOM	1901	N	ALA	A	493	38.275	12.336	14.476	1.00	42.47
ATOM	1902	CA	ALA	A	493	39.570	11.696	14.290	1.00	43.19
ATOM	1903	CB	ALA	A	493	40.374	12.445	13.226	1.00	43.14
ATOM	1904	C	ALA	A	493	40.340	11.640	15.612	1.00	43.40
ATOM	1905	O	ALA	A	493	41.244	10.812	15.802	1.00	44.12
ATOM	1906	N	ILE	A	494	39.979	12.516	16.531	1.00	42.66
ATOM	1907	CA	ILE	A	494	40.651	12.589	17.806	1.00	42.35
ATOM	1908	CB	ILE	A	494	40.873	14.048	18.163	1.00	42.63
ATOM	1909	CG1	ILE	A	494	41.824	14.686	17.155	1.00	44.49
ATOM	1910	CD1	ILE	A	494	41.756	16.198	17.142	1.00	44.88
ATOM	1911	CG2	ILE	A	494	41.451	14.167	19.560	1.00	44.25
ATOM	1912	C	ILE	A	494	39.882	11.920	18.942	1.00	41.61

ATOM	1913	O	ILE	A	494	40.485	11.551	19.953	1.00	41.78
ATOM	1914	N	TYR	A	495	38.566	11.796	18.796	1.00	40.39
ATOM	1915	CA	TYR	A	495	37.722	11.225	19.830	1.00	39.98
ATOM	1916	CB	TYR	A	495	36.916	12.324	20.513	1.00	39.79
ATOM	1917	CG	TYR	A	495	37.731	13.430	21.115	1.00	38.81
ATOM	1918	CD1	TYR	A	495	37.949	14.585	20.415	1.00	38.27
ATOM	1919	CE1	TYR	A	495	38.685	15.600	20.932	1.00	38.45
ATOM	1920	CZ	TYR	A	495	39.209	15.508	22.194	1.00	39.44
ATOM	1921	OH	TYR	A	495	39.947	16.582	22.669	1.00	40.01
ATOM	1922	CE2	TYR	A	495	39.013	14.366	22.941	1.00	38.56
ATOM	1923	CD2	TYR	A	495	38.260	13.329	22.402	1.00	38.69
ATOM	1924	C	TYR	A	495	36.747	10.209	19.257	1.00	40.43
ATOM	1925	O	TYR	A	495	35.548	10.290	19.483	1.00	40.56
ATOM	1926	N	PRO	A	496	37.255	9.201	18.567	1.00	40.98
ATOM	1927	CA	PRO	A	496	36.379	8.261	17.871	1.00	40.62
ATOM	1928	CB	PRO	A	496	37.344	7.229	17.288	1.00	41.12
ATOM	1929	CG	PRO	A	496	38.747	7.789	17.496	1.00	41.49
ATOM	1930	CD	PRO	A	496	38.682	8.848	18.486	1.00	40.68
ATOM	1931	C	PRO	A	496	35.392	7.567	18.796	1.00	40.79
ATOM	1932	O	PRO	A	496	34.263	7.261	18.404	1.00	41.69
ATOM	1933	N	ASP	A	497	35.814	7.254	20.008	1.00	40.89
ATOM	1934	CA	ASP	A	497	34.937	6.528	20.913	1.00	40.80
ATOM	1935	CB	ASP	A	497	35.745	5.792	21.988	1.00	41.84
ATOM	1936	CG	ASP	A	497	36.300	4.475	21.485	1.00	45.64
ATOM	1937	OD1	ASP	A	497	36.821	3.696	22.320	1.00	53.60
ATOM	1938	OD2	ASP	A	497	36.249	4.124	20.282	1.00	48.70
ATOM	1939	C	ASP	A	497	33.902	7.409	21.579	1.00	39.07
ATOM	1940	O	ASP	A	497	32.847	6.919	21.956	1.00	38.09
ATOM	1941	N	ILE	A	498	34.211	8.697	21.744	1.00	38.14
ATOM	1942	CA	ILE	A	498	33.230	9.640	22.273	1.00	37.33
ATOM	1943	CB	ILE	A	498	33.864	11.039	22.491	1.00	38.00
ATOM	1944	CG1	ILE	A	498	34.902	11.018	23.627	1.00	39.27
ATOM	1945	CD1	ILE	A	498	34.375	10.559	24.947	1.00	40.90
ATOM	1946	CG2	ILE	A	498	32.797	12.090	22.770	1.00	37.86
ATOM	1947	C	ILE	A	498	32.092	9.696	21.272	1.00	36.02
ATOM	1948	O	ILE	A	498	30.929	9.572	21.625	1.00	35.72
ATOM	1949	N	VAL	A	499	32.429	9.814	20.002	1.00	35.39
ATOM	1950	CA	VAL	A	499	31.400	9.915	18.994	1.00	35.49
ATOM	1951	CB	VAL	A	499	31.969	10.182	17.580	1.00	34.87
ATOM	1952	CG1	VAL	A	499	30.868	10.168	16.543	1.00	34.58
ATOM	1953	CG2	VAL	A	499	32.686	11.485	17.542	1.00	34.93
ATOM	1954	C	VAL	A	499	30.598	8.647	18.975	1.00	35.88
ATOM	1955	O	VAL	A	499	29.384	8.684	18.933	1.00	36.02
ATOM	1956	N	ARG	A	500	31.278	7.515	19.004	1.00	36.41
ATOM	1957	CA	ARG	A	500	30.600	6.237	18.880	1.00	36.86
ATOM	1958	CB	ARG	A	500	31.629	5.129	18.714	1.00	37.54
ATOM	1959	CG	ARG	A	500	31.058	3.739	18.596	1.00	41.50
ATOM	1960	CD	ARG	A	500	32.137	2.639	18.598	1.00	46.56
ATOM	1961	NE	ARG	A	500	31.814	1.588	19.576	1.00	51.65
ATOM	1962	CZ	ARG	A	500	32.514	1.331	20.688	1.00	52.82
ATOM	1963	NH1	ARG	A	500	33.613	2.013	20.978	1.00	53.74
ATOM	1964	NH2	ARG	A	500	32.117	0.370	21.508	1.00	54.03
ATOM	1965	C	ARG	A	500	29.724	5.950	20.066	1.00	36.07
ATOM	1966	O	ARG	A	500	28.570	5.586	19.884	1.00	36.22
ATOM	1967	N	LEU	A	501	30.247	6.133	21.277	1.00	35.25
ATOM	1968	CA	LEU	A	501	29.493	5.780	22.495	1.00	35.10
ATOM	1969	CB	LEU	A	501	30.444	5.244	23.602	1.00	35.42
ATOM	1970	CG	LEU	A	501	31.187	3.915	23.312	1.00	38.90
ATOM	1971	CD1	LEU	A	501	32.025	3.417	24.493	1.00	41.10
ATOM	1972	CD2	LEU	A	501	30.219	2.807	22.904	1.00	40.70
ATOM	1973	C	LEU	A	501	28.609	6.885	23.083	1.00	33.61
ATOM	1974	O	LEU	A	501	27.660	6.590	23.788	1.00	32.60
ATOM	1975	N	HIS	A	502	28.891	8.152	22.799	1.00	33.08
ATOM	1976	CA	HIS	A	502	28.121	9.226	23.475	1.00	32.46
ATOM	1977	CB	HIS	A	502	29.049	9.936	24.480	1.00	32.21
ATOM	1978	CG	HIS	A	502	29.690	8.993	25.454	1.00	32.45

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ATOM	1979	ND1	HIS	A	502	28.998	8.440	26.515	1.00	34.45	N
ATOM	1980	CE1	HIS	A	502	29.796	7.616	27.175	1.00	33.23	C
ATOM	1981	NE2	HIS	A	502	30.978	7.610	26.582	1.00	32.06	N
ATOM	1982	CD2	HIS	A	502	30.940	8.457	25.499	1.00	32.50	C
ATOM	1983	C	HIS	A	502	27.392	10.237	22.575	1.00	31.35	C
ATOM	1984	O	HIS	A	502	26.671	11.084	23.064	1.00	32.31	O
ATOM	1985	N	PHE	A	503	27.572	10.171	21.269	1.00	30.30	N
ATOM	1986	CA	PHE	A	503	26.839	11.071	20.401	1.00	29.71	C
ATOM	1987	CB	PHE	A	503	27.636	11.366	19.123	1.00	28.59	C
ATOM	1988	CG	PHE	A	503	28.589	12.527	19.253	1.00	27.67	C
ATOM	1989	CD1	PHE	A	503	29.265	12.774	20.443	1.00	28.62	C
ATOM	1990	CE1	PHE	A	503	30.132	13.869	20.575	1.00	24.57	C
ATOM	1991	CZ	PHE	A	503	30.313	14.715	19.523	1.00	23.93	C
ATOM	1992	CE2	PHE	A	503	29.635	14.481	18.322	1.00	27.80	C
ATOM	1993	CD2	PHE	A	503	28.783	13.402	18.194	1.00	27.49	C
ATOM	1994	C	PHE	A	503	25.465	10.483	20.086	1.00	29.88	C
ATOM	1995	O	PHE	A	503	25.301	9.290	20.004	1.00	29.58	O
ATOM	1996	N	PRO	A	504	24.472	11.327	19.887	1.00	30.28	N
ATOM	1997	CA	PRO	A	504	23.131	10.838	19.561	1.00	30.42	C
ATOM	1998	CB	PRO	A	504	22.305	12.107	19.435	1.00	30.02	C
ATOM	1999	CG	PRO	A	504	23.129	13.163	20.095	1.00	30.50	C
ATOM	2000	CD	PRO	A	504	24.559	12.793	19.900	1.00	29.70	C
ATOM	2001	C	PRO	A	504	23.112	10.094	18.232	1.00	30.68	C
ATOM	2002	O	PRO	A	504	23.698	10.533	17.261	1.00	29.79	O
ATOM	2003	N	PRO	A	505	22.410	8.973	18.199	1.00	31.99	N
ATOM	2004	CA	PRO	A	505	22.330	8.126	16.997	1.00	32.55	C
ATOM	2005	CB	PRO	A	505	21.334	7.055	17.397	1.00	32.91	C
ATOM	2006	CG	PRO	A	505	21.520	6.943	18.876	1.00	33.39	C
ATOM	2007	CD	PRO	A	505	21.710	8.384	19.347	1.00	32.17	C
ATOM	2008	C	PRO	A	505	21.866	8.820	15.736	1.00	32.64	C
ATOM	2009	O	PRO	A	505	22.416	8.540	14.662	1.00	33.22	O
ATOM	2010	N	LEU	A	506	20.888	9.709	15.843	1.00	32.69	N
ATOM	2011	CA	LEU	A	506	20.388	10.427	14.673	1.00	32.07	C
ATOM	2012	CB	LEU	A	506	19.117	11.204	15.015	1.00	32.44	C
ATOM	2013	CG	LEU	A	506	18.566	12.012	13.840	1.00	31.16	C
ATOM	2014	CD1	LEU	A	506	18.156	11.092	12.722	1.00	33.03	C
ATOM	2015	CD2	LEU	A	506	17.398	12.836	14.302	1.00	32.49	C
ATOM	2016	C	LEU	A	506	21.425	11.369	14.091	1.00	32.28	C
ATOM	2017	O	LEU	A	506	21.491	11.528	12.893	1.00	32.61	O
ATOM	2018	N	TYR	A	507	22.210	12.012	14.949	1.00	32.83	N
ATOM	2019	CA	TYR	A	507	23.327	12.879	14.533	1.00	32.73	C
ATOM	2020	CB	TYR	A	507	23.927	13.589	15.762	1.00	32.18	C
ATOM	2021	CG	TYR	A	507	25.025	14.643	15.516	1.00	30.21	C
ATOM	2022	CD1	TYR	A	507	24.733	15.980	15.458	1.00	27.51	C
ATOM	2023	CE1	TYR	A	507	25.715	16.908	15.284	1.00	28.26	C
ATOM	2024	CZ	TYR	A	507	27.020	16.500	15.176	1.00	29.93	C
ATOM	2025	OH	TYR	A	507	28.032	17.414	14.997	1.00	30.78	O
ATOM	2026	CE2	TYR	A	507	27.336	15.180	15.239	1.00	28.89	C
ATOM	2027	CD2	TYR	A	507	26.365	14.273	15.423	1.00	29.57	C
ATOM	2028	C	TYR	A	507	24.405	12.054	13.802	1.00	33.67	C
ATOM	2029	O	TYR	A	507	24.928	12.468	12.770	1.00	32.52	O
ATOM	2030	N	LYS	A	508	24.730	10.895	14.351	1.00	35.19	N
ATOM	2031	CA	LYS	A	508	25.674	9.979	13.703	1.00	36.84	C
ATOM	2032	CB	LYS	A	508	25.931	8.740	14.548	1.00	36.89	C
ATOM	2033	CG	LYS	A	508	26.837	8.988	15.763	1.00	38.78	C
ATOM	2034	CD	LYS	A	508	27.446	7.686	16.296	1.00	39.11	C
ATOM	2035	CE	LYS	A	508	26.536	7.042	17.265	1.00	41.23	C
ATOM	2036	NZ	LYS	A	508	27.053	5.702	17.721	1.00	42.04	N
ATOM	2037	C	LYS	A	508	25.165	9.560	12.332	1.00	37.51	C
ATOM	2038	O	LYS	A	508	25.908	9.643	11.386	1.00	37.79	O
ATOM	2039	N	GLU	A	509	23.893	9.165	12.232	1.00	38.63	N
ATOM	2040	CA	GLU	A	509	23.313	8.734	10.968	1.00	39.31	C
ATOM	2041	CB	GLU	A	509	21.863	8.281	11.131	1.00	39.58	C
ATOM	2042	CG	GLU	A	509	21.670	6.932	11.815	1.00	44.44	C
ATOM	2043	CD	GLU	A	509	20.198	6.514	11.993	1.00	48.40	C
ATOM	2044	OE1	GLU	A	509	19.956	5.642	12.854	1.00	52.15	O



ATOM	2045	OE2	GLU	A	509	19.285	7.028	11.285	1.00	50.58	O
ATOM	2046	C	GLU	A	509	23.333	9.841	9.937	1.00	39.53	C
ATOM	2047	O	GLU	A	509	23.504	9.571	8.745	1.00	39.45	O
ATOM	2048	N	LEU	A	510	23.126	11.083	10.379	1.00	39.18	N
ATOM	2049	CA	LEU	A	510	23.067	12.201	9.456	1.00	39.07	C
ATOM	2050	CB	LEU	A	510	22.226	13.338	10.040	1.00	39.33	C
ATOM	2051	CG	LEU	A	510	20.725	13.091	10.200	1.00	39.95	C
ATOM	2052	CD1	LEU	A	510	20.091	14.296	10.800	1.00	41.52	C
ATOM	2053	CD2	LEU	A	510	20.058	12.768	8.899	1.00	40.94	C
ATOM	2054	C	LEU	A	510	24.401	12.783	9.030	1.00	38.89	C
ATOM	2055	O	LEU	A	510	24.503	13.334	7.943	1.00	39.03	O
ATOM	2056	N	PHE	A	511	25.427	12.680	9.854	1.00	38.62	N
ATOM	2057	CA	PHE	A	511	26.619	13.464	9.591	1.00	38.51	C
ATOM	2058	CB	PHE	A	511	26.736	14.569	10.646	1.00	38.47	C
ATOM	2059	CG	PHE	A	511	25.542	15.483	10.711	1.00	39.17	C
ATOM	2060	CD1	PHE	A	511	24.848	15.663	11.910	1.00	37.90	C
ATOM	2061	CE1	PHE	A	511	23.762	16.508	11.985	1.00	37.16	C
ATOM	2062	CZ	PHE	A	511	23.324	17.165	10.866	1.00	39.02	C
ATOM	2063	CE2	PHE	A	511	24.005	16.998	9.653	1.00	39.88	C
ATOM	2064	CD2	PHE	A	511	25.113	16.167	9.587	1.00	40.32	C
ATOM	2065	C	PHE	A	511	27.915	12.682	9.565	1.00	38.68	C
ATOM	2066	O	PHE	A	511	28.923	13.297	9.211	1.00	38.22	O
ATOM	2067	OXT	PHE	A	511	27.963	11.489	9.895	1.00	39.77	O
ATOM	2068	C65	CHS	L	1	29.670	21.352	16.280	1.00	40.20	C
ATOM	2069	C63	CHS	L	1	28.173	21.713	16.502	1.00	35.49	C
ATOM	2070	C69	CHS	L	1	27.552	20.583	17.354	1.00	36.38	C
ATOM	2071	C60	CHS	L	1	28.076	23.102	17.181	1.00	33.50	C
ATOM	2072	C57	CHS	L	1	26.755	23.921	17.026	1.00	29.77	C
ATOM	2073	C54	CHS	L	1	26.543	24.885	18.224	1.00	26.05	C
ATOM	2074	C48	CHS	L	1	25.339	25.868	18.122	1.00	27.06	C
ATOM	2075	C50	CHS	L	1	25.416	26.630	16.786	1.00	30.39	C
ATOM	2076	C38	CHS	L	1	23.999	25.113	18.108	1.00	27.35	C
ATOM	2077	C35	CHS	L	1	23.898	24.161	19.333	1.00	25.32	C
ATOM	2078	C29	CHS	L	1	22.637	25.885	18.088	1.00	25.81	C
ATOM	2079	C26	CHS	L	1	22.075	26.442	16.760	1.00	25.48	C
ATOM	2080	C40	CHS	L	1	22.674	27.065	19.089	1.00	24.66	C
ATOM	2081	C30	CHS	L	1	21.683	24.733	18.480	1.00	24.66	C
ATOM	2082	C32	CHS	L	1	22.378	23.988	19.639	1.00	25.34	C
ATOM	2083	C18	CHS	L	1	20.267	25.269	18.823	1.00	24.65	C
ATOM	2084	C15	CHS	L	1	19.389	24.126	19.379	1.00	27.21	C
ATOM	2085	C20	CHS	L	1	19.656	25.910	17.559	1.00	25.94	C
ATOM	2086	C23	CHS	L	1	20.616	26.987	16.956	1.00	25.70	C
ATOM	2087	C22	CHS	L	1	18.195	26.423	17.788	1.00	25.96	C
ATOM	2088	C44	CHS	L	1	18.216	27.828	18.461	1.00	23.41	C
ATOM	2089	C12	CHS	L	1	17.391	25.437	18.627	1.00	27.66	C
ATOM	2090	C9	CHS	L	1	15.878	25.602	18.705	1.00	27.52	C
ATOM	2091	C13	CHS	L	1	17.928	24.439	19.343	1.00	28.47	C
ATOM	2092	C1	CHS	L	1	17.457	26.540	16.432	1.00	24.95	C
ATOM	2093	C4	CHS	L	1	15.966	26.932	16.596	1.00	25.61	C
ATOM	2094	C7	CHS	L	1	15.184	25.850	17.366	1.00	27.22	C
ATOM	2095	O6	CHS	L	1	13.884	26.323	17.783	1.00	33.31	O
ATOM	2096	S1	CHS	L	1	12.600	26.109	16.995	1.00	36.30	S
ATOM	2097	O3	CHS	L	1	11.492	26.689	17.749	1.00	35.79	O
ATOM	2098	O2	CHS	L	1	12.386	24.736	16.612	1.00	34.23	O
ATOM	2099	O4	CHS	L	1	12.791	26.916	15.768	1.00	31.69	O
ATOM	2100	O	HOH	V	1	34.374	18.778	31.636	1.00	24.18	O
ATOM	2101	O	HOH	V	2	13.751	22.827	14.717	1.00	25.05	O
ATOM	2102	O	HOH	V	3	17.585	18.928	1.035	1.00	25.61	O
ATOM	2103	O	HOH	V	4	19.468	24.062	23.227	1.00	25.84	O
ATOM	2104	O	HOH	V	5	28.242	16.854	27.596	1.00	28.05	O
ATOM	2105	O	HOH	V	6	26.219	37.914	34.970	1.00	28.23	O
ATOM	2106	O	HOH	V	7	25.424	34.243	27.348	1.00	29.16	O
ATOM	2107	O	HOH	V	8	37.940	8.815	22.096	1.00	29.22	O
ATOM	2108	O	HOH	V	9	34.532	27.583	19.498	1.00	30.78	O
ATOM	2109	O	HOH	V	10	36.533	26.810	13.236	1.00	30.95	O
ATOM	2110	O	HOH	V	11	19.929	34.372	33.559	1.00	31.12	O

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ATOM	2111	O	HOH	V	12	30.464	36.924	16.913	1.00	32.33	O
ATOM	2112	O	HOH	V	13	39.694	19.997	26.277	1.00	32.46	O
ATOM	2113	O	HOH	V	14	10.618	25.915	9.224	1.00	33.09	O
ATOM	2114	O	HOH	V	15	19.089	15.060	21.458	1.00	33.35	O
ATOM	2115	O	HOH	V	16	19.982	38.502	24.574	1.00	33.56	O
ATOM	2116	O	HOH	V	17	29.188	18.773	31.889	1.00	34.82	O
ATOM	2117	O	HOH	V	18	32.816	26.367	25.939	1.00	35.28	O
ATOM	2118	O	HOH	V	19	21.757	13.531	27.380	1.00	35.38	O
ATOM	2119	O	HOH	V	20	21.923	18.531	7.233	1.00	35.96	O
ATOM	2120	O	HOH	V	21	33.494	32.602	17.864	1.00	36.22	O
ATOM	2121	O	HOH	V	22	29.529	39.171	20.916	1.00	36.73	O
ATOM	2122	O	HOH	V	23	26.956	19.335	8.080	1.00	37.09	O
ATOM	2123	O	HOH	V	24	17.942	26.092	21.769	1.00	37.19	O
ATOM	2124	O	HOH	V	25	30.129	36.843	14.123	1.00	37.60	O
ATOM	2125	O	HOH	V	26	26.979	35.078	38.228	1.00	37.66	O
ATOM	2126	O	HOH	V	27	11.702	12.320	-11.449	1.00	37.83	O
ATOM	2127	O	HOH	V	28	24.019	40.426	26.459	1.00	38.20	O
ATOM	2128	O	HOH	V	29	32.889	38.167	8.976	1.00	38.30	O
ATOM	2129	O	HOH	V	30	26.368	37.122	27.563	1.00	38.38	O
ATOM	2130	O	HOH	V	31	26.038	37.728	37.444	1.00	38.65	O
ATOM	2131	O	HOH	V	32	-0.184	22.111	6.895	1.00	38.91	O
ATOM	2132	O	HOH	V	33	24.132	19.988	-1.108	1.00	39.60	O
ATOM	2133	O	HOH	V	34	17.228	26.642	24.728	1.00	39.66	O
ATOM	2134	O	HOH	V	35	24.430	17.401	-1.616	1.00	40.07	O
ATOM	2135	O	HOH	V	36	14.466	37.465	9.931	1.00	40.09	O
ATOM	2136	O	HOH	V	37	38.590	23.562	23.909	1.00	40.15	O
ATOM	2137	O	HOH	V	38	20.064	26.866	31.634	1.00	40.16	O
ATOM	2138	O	HOH	V	39	5.285	36.507	11.739	1.00	40.86	O
ATOM	2139	O	HOH	V	40	5.515	30.530	16.484	1.00	40.87	O
ATOM	2140	O	HOH	V	41	24.115	12.660	27.541	1.00	40.92	O
ATOM	2141	O	HOH	V	42	23.756	5.602	14.704	1.00	41.17	O
ATOM	2142	O	HOH	V	43	10.524	40.707	27.825	1.00	41.34	O
ATOM	2143	O	HOH	V	44	26.115	7.036	20.648	1.00	41.58	O
ATOM	2144	O	HOH	V	45	22.909	14.371	0.739	1.00	41.86	O
ATOM	2145	O	HOH	V	46	38.001	12.389	26.816	1.00	42.12	O
ATOM	2146	O	HOH	V	47	27.038	38.349	22.646	1.00	42.13	O
ATOM	2147	O	HOH	V	48	27.926	38.210	14.696	1.00	42.24	O
ATOM	2148	O	HOH	V	49	19.208	17.322	27.275	1.00	42.36	O
ATOM	2149	O	HOH	V	50	17.702	22.996	26.002	1.00	42.43	O
ATOM	2150	O	HOH	V	51	21.518	40.403	26.071	1.00	42.44	O
ATOM	2151	O	HOH	V	52	29.008	37.276	26.773	1.00	42.97	O
ATOM	2152	O	HOH	V	53	16.797	40.023	17.063	1.00	43.20	O
ATOM	2153	O	HOH	V	54	27.959	18.192	30.078	1.00	43.25	O
ATOM	2154	O	HOH	V	55	27.189	38.094	30.644	1.00	43.31	O
ATOM	2155	O	HOH	V	56	32.853	5.119	27.654	1.00	43.36	O
ATOM	2156	O	HOH	V	57	25.498	15.066	28.345	1.00	43.59	O
ATOM	2157	O	HOH	V	58	26.277	3.798	24.349	1.00	43.69	O
ATOM	2158	O	HOH	V	59	24.431	4.474	16.791	1.00	43.83	O
ATOM	2159	O	HOH	V	60	17.931	21.585	22.061	1.00	43.86	O
ATOM	2160	O	HOH	V	61	3.622	36.866	6.230	1.00	43.90	O
ATOM	2161	O	HOH	V	62	29.565	0.033	25.439	1.00	44.03	O
ATOM	2162	O	HOH	V	63	37.471	27.196	26.904	1.00	44.11	O
ATOM	2163	O	HOH	V	64	14.114	35.615	19.648	1.00	44.14	O
ATOM	2164	O	HOH	V	65	32.375	30.570	3.935	1.00	44.29	O
ATOM	2165	O	HOH	V	66	23.674	14.801	-1.168	1.00	44.29	O
ATOM	2166	O	HOH	V	67	10.607	41.218	4.126	1.00	44.59	O
ATOM	2167	O	HOH	V	68	5.553	22.195	-4.232	1.00	45.31	O
ATOM	2168	O	HOH	V	69	18.683	8.716	-3.851	1.00	45.45	O
ATOM	2169	O	HOH	V	70	31.216	36.554	23.614	1.00	45.65	O
ATOM	2170	O	HOH	V	71	32.042	38.382	12.898	1.00	45.78	O
ATOM	2171	O	HOH	V	72	41.571	18.538	20.942	1.00	45.85	O
ATOM	2172	O	HOH	V	73	24.529	18.718	30.164	1.00	45.93	O
ATOM	2173	O	HOH	V	74	12.539	36.492	16.322	1.00	45.97	O
ATOM	2174	O	HOH	V	75	41.603	15.767	13.285	1.00	46.25	O
ATOM	2175	O	HOH	V	76	21.193	17.911	28.154	1.00	46.47	O
ATOM	2176	O	HOH	V	77	29.518	22.554	36.275	1.00	46.60	O

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ATOM	2177	O	HOH V	78	32.636	35.308	17.598	1.00	47.00	O
ATOM	2178	O	HOH V	79	13.479	40.537	21.946	1.00	47.13	O
ATOM	2179	O	HOH V	80	32.129	25.488	3.702	1.00	47.21	O
ATOM	2180	O	HOH V	81	5.317	15.523	10.878	1.00	47.24	O
ATOM	2181	O	HOH V	82	14.590	12.994	-13.138	1.00	47.42	O
ATOM	2182	O	HOH V	83	31.688	18.521	32.632	1.00	47.42	O
ATOM	2183	O	HOH V	84	17.527	41.724	24.627	1.00	47.58	O
ATOM	2184	O	HOH V	85	2.758	27.645	-6.136	1.00	47.76	O
ATOM	2185	O	HOH V	86	39.479	15.402	9.361	1.00	47.77	O
ATOM	2186	O	HOH V	87	27.097	39.457	7.716	1.00	47.80	O
ATOM	2187	O	HOH V	88	14.854	38.493	18.833	1.00	48.18	O
ATOM	2188	O	HOH V	89	16.442	28.965	31.902	1.00	48.22	O
ATOM	2189	O	HOH V	90	6.592	18.094	16.102	1.00	48.28	O
ATOM	2190	O	HOH V	91	25.862	43.114	20.667	1.00	48.28	O
ATOM	2191	O	HOH V	92	25.820	31.283	38.083	1.00	48.37	O
ATOM	2192	O	HOH V	93	21.448	8.215	-6.909	1.00	48.43	O
ATOM	2193	O	HOH V	94	30.315	7.953	13.447	1.00	48.47	O
ATOM	2194	O	HOH V	95	11.333	3.609	-1.448	1.00	48.50	O
ATOM	2195	O	HOH V	96	25.475	26.684	-3.988	1.00	48.54	O
ATOM	2196	O	HOH V	97	21.825	7.068	6.249	1.00	48.57	O
ATOM	2197	O	HOH V	98	26.277	39.627	9.743	1.00	48.67	O
ATOM	2198	O	HOH V	99	10.637	33.053	31.840	1.00	48.70	O
ATOM	2199	O	HOH V	100	8.248	10.674	15.177	1.00	48.90	O
ATOM	2200	O	HOH V	101	5.925	25.750	18.970	1.00	48.97	O
ATOM	2201	O	HOH V	102	15.403	29.322	-7.859	1.00	49.09	O
ATOM	2202	O	HOH V	103	3.536	35.057	9.239	1.00	49.16	O
ATOM	2203	O	HOH V	104	24.615	19.046	6.759	1.00	49.20	O
ATOM	2204	O	HOH V	105	26.458	22.354	32.348	1.00	49.22	O
ATOM	2205	O	HOH V	106	29.329	9.438	8.558	1.00	49.24	O
ATOM	2206	O	HOH V	107	38.968	26.081	25.260	1.00	49.30	O
ATOM	2207	O	HOH V	108	33.166	31.078	20.463	1.00	49.55	O
ATOM	2208	O	HOH V	109	23.661	41.348	9.046	1.00	49.57	O
ATOM	2209	O	HOH V	110	-1.905	38.422	-2.103	1.00	49.58	O
ATOM	2210	O	HOH V	111	23.567	25.829	32.172	1.00	49.84	O
ATOM	2211	O	HOH V	112	39.174	28.173	18.167	1.00	49.89	O
ATOM	2212	O	HOH V	113	6.546	17.330	-8.809	1.00	50.15	O
ATOM	2213	O	HOH V	114	15.378	36.610	16.329	1.00	50.24	O
ATOM	2214	O	HOH V	115	24.014	21.545	30.393	1.00	50.25	O
ATOM	2215	O	HOH V	116	13.119	40.412	25.848	1.00	50.51	O
ATOM	2216	O	HOH V	117	34.344	32.657	10.572	1.00	50.99	O
ATOM	2217	O	HOH V	118	26.462	26.162	35.827	1.00	51.01	O
ATOM	2218	O	HOH V	119	37.119	20.213	15.138	1.00	51.01	O
ATOM	2219	O	HOH V	120	20.402	7.809	0.264	1.00	51.21	O
ATOM	2220	O	HOH V	121	32.907	23.096	33.511	1.00	51.26	O
ATOM	2221	O	HOH V	122	18.316	15.239	25.933	1.00	51.36	O
ATOM	2222	O	HOH V	123	22.210	27.272	33.235	1.00	51.39	O
ATOM	2223	O	HOH V	124	4.773	34.446	-7.751	1.00	51.56	O
ATOM	2224	O	HOH V	125	-11.176	24.480	-12.026	1.00	51.70	O
ATOM	2225	O	HOH V	126	29.201	40.901	16.488	1.00	51.72	O
ATOM	2226	O	HOH V	127	-14.169	32.191	-15.792	1.00	51.83	O
ATOM	2227	O	HOH V	128	27.174	21.751	2.087	1.00	51.83	O
ATOM	2228	O	HOH V	129	12.661	30.921	30.244	1.00	51.89	O
ATOM	2229	O	HOH V	130	16.175	21.212	25.031	1.00	51.93	O
ATOM	2230	O	HOH V	131	20.211	40.398	29.373	1.00	52.00	O
ATOM	2231	O	HOH V	132	-13.899	29.982	-18.098	1.00	52.10	O
ATOM	2232	O	HOH V	133	15.844	9.719	16.408	1.00	52.40	O
ATOM	2233	O	HOH V	134	31.386	39.552	17.146	1.00	52.59	O
ATOM	2234	O	HOH V	135	0.640	32.016	4.846	1.00	52.62	O
ATOM	2235	O	HOH V	136	42.270	20.847	16.516	1.00	52.68	O
ATOM	2236	O	HOH V	137	17.490	42.697	21.680	1.00	52.79	O
ATOM	2237	O	HOH V	138	29.839	40.760	8.920	1.00	52.82	O
ATOM	2238	O	HOH V	139	4.290	30.109	9.865	1.00	52.89	O
ATOM	2239	O	HOH V	140	19.892	7.267	-2.229	1.00	53.00	O
ATOM	2240	O	HOH V	141	9.212	35.423	31.648	1.00	53.10	O
ATOM	2241	O	HOH V	142	31.957	28.820	37.099	1.00	53.23	O
ATOM	2242	O	HOH V	143	40.970	31.344	14.438	1.00	53.27	O

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ATOM	2243	O	HOH	V	144	40.782	22.485	20.153	1.00	53.41	O
ATOM	2244	O	HOH	V	145	4.688	33.007	-12.475	1.00	53.62	O
ATOM	2245	O	HOH	V	146	12.405	42.730	-6.583	1.00	53.65	O
ATOM	2246	O	HOH	V	147	30.118	41.753	23.343	1.00	53.90	O
ATOM	2247	O	HOH	V	148	40.310	19.731	15.626	1.00	54.03	O
ATOM	2248	O	HOH	V	149	9.904	10.991	-10.125	1.00	54.05	O
ATOM	2249	O	HOH	V	150	35.645	26.966	10.324	1.00	54.10	O
ATOM	2250	O	HOH	V	151	3.249	13.849	9.818	1.00	54.12	O
ATOM	2251	O	HOH	V	152	8.994	41.917	8.500	1.00	54.13	O
ATOM	2252	O	HOH	V	153	25.494	7.351	8.323	1.00	54.13	O
ATOM	2253	O	HOH	V	154	-19.853	30.788	-6.983	1.00	54.14	O
ATOM	2254	O	HOH	V	155	28.190	2.825	26.243	1.00	54.20	O
ATOM	2255	O	HOH	V	156	14.754	37.385	13.109	1.00	54.33	O
ATOM	2256	O	HOH	V	157	13.944	9.467	-11.887	1.00	54.33	O
ATOM	2257	O	HOH	V	158	5.602	27.878	16.557	1.00	54.52	O
ATOM	2258	O	HOH	V	159	35.605	5.102	13.754	1.00	54.70	O
ATOM	2259	O	HOH	V	160	24.308	35.094	-1.504	1.00	54.70	O
ATOM	2260	O	HOH	V	161	28.337	18.154	4.417	1.00	54.85	O
ATOM	2261	O	HOH	V	162	34.895	34.791	30.514	1.00	54.94	O
ATOM	2262	O	HOH	V	163	4.910	16.781	14.763	1.00	55.00	O
ATOM	2263	O	HOH	V	164	11.023	5.038	5.200	1.00	55.13	O
ATOM	2264	O	HOH	V	165	39.542	17.117	25.841	1.00	55.21	O
ATOM	2265	O	HOH	V	166	24.386	37.780	-6.091	1.00	55.24	O
ATOM	2266	O	HOH	V	167	20.889	19.941	29.200	1.00	55.34	O
ATOM	2267	O	HOH	V	168	6.752	22.057	-14.805	1.00	55.38	O
ATOM	2268	O	HOH	V	169	25.163	5.963	12.276	1.00	55.50	O
ATOM	2269	O	HOH	V	170	28.609	39.754	12.521	1.00	55.51	O
ATOM	2270	O	HOH	V	171	11.031	13.390	14.244	1.00	55.56	O
ATOM	2271	O	HOH	V	172	24.662	35.439	2.257	1.00	55.60	O
ATOM	2272	O	HOH	V	173	36.161	34.403	25.458	1.00	55.61	O
ATOM	2273	O	HOH	V	174	9.631	6.595	3.959	1.00	55.62	O
ATOM	2274	O	HOH	V	175	38.038	17.337	8.038	1.00	55.79	O
ATOM	2275	O	HOH	V	176	0.834	36.938	9.105	1.00	55.88	O
ATOM	2276	O	HOH	V	177	30.977	6.285	15.282	1.00	55.89	O
ATOM	2277	O	HOH	V	178	36.456	34.296	14.233	1.00	55.99	O
ATOM	2278	O	HOH	V	179	-16.740	27.510	-6.376	1.00	56.17	O
ATOM	2279	O	HOH	V	180	17.830	28.498	-7.217	1.00	56.32	O
ATOM	2280	O	HOH	V	181	27.092	42.066	23.041	1.00	56.37	O
ATOM	2281	O	HOH	V	182	32.854	20.918	3.041	1.00	56.40	O
ATOM	2282	O	HOH	V	183	33.531	36.555	20.279	1.00	56.52	O
ATOM	2283	O	HOH	V	184	29.161	9.790	11.459	1.00	56.74	O
ATOM	2284	O	HOH	V	185	30.947	21.061	33.802	1.00	56.78	O
ATOM	2285	O	HOH	V	186	4.419	10.917	12.329	1.00	57.20	O
ATOM	2286	O	HOH	V	187	35.731	21.349	33.562	1.00	57.25	O
ATOM	2287	O	HOH	V	188	10.127	34.435	-7.921	1.00	57.31	O
ATOM	2288	O	HOH	V	189	24.815	39.636	5.433	1.00	57.31	O
ATOM	2289	O	HOH	V	190	16.135	28.959	-10.450	1.00	57.40	O
ATOM	2290	O	HOH	V	191	28.755	27.074	-0.804	1.00	57.58	O
ATOM	2291	O	HOH	V	192	37.694	28.335	20.845	1.00	58.09	O
ATOM	2292	O	HOH	V	193	12.094	17.839	22.662	1.00	58.11	O
ATOM	2293	O	HOH	V	194	16.739	12.034	-12.326	1.00	58.15	O
ATOM	2294	O	HOH	V	195	35.658	34.834	39.271	1.00	58.17	O
ATOM	2295	O	HOH	V	196	6.325	23.731	-10.962	1.00	58.22	O
ATOM	2296	O	HOH	V	197	40.239	32.219	19.158	1.00	58.22	O
ATOM	2297	O	HOH	V	198	42.009	17.600	28.618	1.00	58.40	O
ATOM	2298	O	HOH	V	199	13.977	43.767	4.977	1.00	58.43	O
ATOM	2299	O	HOH	V	200	16.099	2.261	-8.711	1.00	58.43	O
ATOM	2300	O	HOH	V	201	28.967	4.492	15.572	1.00	58.44	O
ATOM	2301	O	HOH	V	202	-9.860	29.231	-7.273	1.00	58.50	O
ATOM	2302	O	HOH	V	203	19.071	45.087	23.986	1.00	58.89	O
ATOM	2303	O	HOH	V	204	23.529	32.968	-5.882	1.00	59.37	O
ATOM	2304	O	HOH	V	205	42.799	19.843	29.263	1.00	59.50	O
ATOM	2305	O	HOH	V	206	21.137	24.412	31.357	1.00	59.65	O
ATOM	2306	O	HOH	V	207	21.855	22.367	32.296	1.00	59.84	O
ATOM	2307	O	HOH	V	208	3.008	31.149	11.774	1.00	59.88	O
ATOM	2308	O	HOH	V	209	25.290	39.928	29.735	1.00	59.89	O

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ATOM	2309	O	HOH V 210	20.546	26.076	-5.981	1.00	60.27	O
ATOM	2310	O	HOH V 211	7.922	7.232	-0.636	1.00	60.32	O
ATOM	2311	O	HOH V 212	7.268	35.864	-11.540	1.00	60.42	O
ATOM	2312	O	HOH V 213	5.789	26.044	-10.740	1.00	60.43	O
ATOM	2313	O	HOH V 214	26.552	14.136	-0.935	1.00	60.54	O
ATOM	2314	O	HOH V 215	41.103	32.645	22.002	1.00	60.87	O
ATOM	2315	O	HOH V 216	10.211	45.156	8.475	1.00	61.19	O
ATOM	2316	O	HOH V 217	25.176	9.626	5.053	1.00	61.26	O
ATOM	2317	O	HOH V 218	11.154	41.223	20.664	1.00	61.36	O
ATOM	2318	O	HOH V 219	12.673	39.495	16.829	1.00	61.48	O
ATOM	2319	O	HOH V 220	6.931	21.130	20.882	1.00	61.81	O
ATOM	2320	O	HOH V 221	34.324	35.314	27.782	1.00	61.99	O
ATOM	2321	O	HOH V 222	22.533	27.773	-4.889	1.00	62.36	O
ATOM	2322	O	HOH V 223	26.615	24.563	-3.514	1.00	62.43	O
ATOM	2323	O	HOH V 224	22.620	8.612	-0.252	1.00	62.66	O
ATOM	2324	O	HOH V 225	7.850	40.686	5.273	1.00	62.89	O
ATOM	2325	O	HOH V 226	13.072	10.222	19.270	1.00	62.97	O
ATOM	2326	O	HOH V 227	36.863	23.365	8.281	1.00	63.29	O
ATOM	2327	O	HOH V 228	3.086	21.555	0.662	1.00	63.45	O
ATOM	2328	O	HOH V 229	40.090	16.185	28.416	1.00	63.62	O
ATOM	2329	O	HOH V 230	28.499	41.692	20.652	1.00	63.74	O
ATOM	2330	O	HOH V 231	5.053	21.524	-0.933	1.00	63.76	O
ATOM	2331	O	HOH V 232	18.279	22.767	-9.711	1.00	63.86	O
ATOM	2332	O	HOH V 233	4.021	13.207	14.475	1.00	64.13	O
ATOM	2333	O	HOH V 234	20.707	46.785	18.023	1.00	64.17	O
ATOM	2334	O	HOH V 235	18.269	24.266	-5.185	1.00	64.61	O
ATOM	2335	O	HOH V 236	-1.075	31.083	6.459	1.00	64.71	O
ATOM	2336	O	HOH V 237	36.067	6.771	10.766	1.00	64.72	O
ATOM	2337	O	HOH V 238	41.379	11.059	22.312	1.00	64.85	O
ATOM	2338	O	HOH V 239	2.764	21.069	-4.139	1.00	64.89	O
ATOM	2339	O	HOH V 240	36.774	12.493	29.500	1.00	64.91	O
ATOM	2340	O	HOH V 241	33.576	7.054	15.865	1.00	65.14	O
ATOM	2341	O	HOH V 242	14.783	25.737	26.607	1.00	65.39	O
ATOM	2342	O	HOH V 243	19.632	29.934	-8.079	1.00	65.40	O
ATOM	2343	O	HOH V 244	19.893	42.353	12.315	1.00	65.64	O
ATOM	2344	O	HOH V 245	30.511	40.345	32.883	1.00	66.15	O
ATOM	2345	O	HOH V 246	6.494	31.838	-13.514	1.00	66.20	O
ATOM	2346	O	HOH V 247	41.592	29.824	26.952	1.00	67.14	O
ATOM	2347	O	HOH V 248	10.095	12.965	-13.010	1.00	68.08	O
ATOM	2348	O	HOH V 249	28.076	13.999	7.164	1.00	68.53	O
ATOM	2349	O	HOH V 250	16.142	3.364	3.323	1.00	68.80	O
ATOM	2350	O	HOH V 251	11.453	41.019	-1.487	1.00	68.99	O
ATOM	2351	O	HOH V 252	22.049	30.697	36.943	1.00	69.14	O
ATOM	2352	O	HOH V 253	31.306	29.631	39.320	1.00	69.25	O
ATOM	2353	O	HOH V 254	26.120	35.578	0.298	1.00	69.34	O
ATOM	2354	O	HOH V 255	37.240	33.402	37.433	1.00	69.56	O
ATOM	2355	O	HOH V 256	14.450	19.763	22.059	1.00	70.09	O